

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
 Data File : BN033384.D
 Acq On : 14 Aug 2024 15:57
 Operator : MA/JU
 Sample : P3502-21
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 DCXV5

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BN033384.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.405	67	71	81	rBV	215466	314209	1.50%	0.216%
2	3.546	91	95	107	rBV	136343	200766	0.96%	0.138%
3	5.693	450	460	469	rBV	56573	92723	0.44%	0.064%
4	6.287	555	561	569	rVB	1052988	1591147	7.61%	1.095%
5	6.587	606	612	616	rBV	102281	162150	0.78%	0.112%
6	6.752	628	640	649	rBV	1075338	1718064	8.21%	1.183%
7	6.916	657	668	676	rBV	790382	1181319	5.65%	0.813%
8	7.028	681	687	691	rVV	106698	166364	0.80%	0.115%
9	7.105	695	700	709	rVV	1042173	1572617	7.52%	1.083%
10	7.181	709	713	725	rVB	58881	94541	0.45%	0.065%
11	7.569	770	779	787	rBV	1225499	1868225	8.93%	1.286%
12	8.269	889	898	909	rBV	1244340	1973255	9.43%	1.358%
13	8.710	965	973	980	rBV	934536	1513964	7.24%	1.042%
14	9.287	1065	1071	1078	rBV	182337	281487	1.35%	0.194%
15	9.422	1085	1094	1102	rBV	745298	1213400	5.80%	0.835%
16	9.575	1111	1120	1130	rBV	72900	158572	0.76%	0.109%
17	9.957	1178	1185	1196	rBV	1359434	2260842	10.81%	1.556%
18	10.334	1242	1249	1256	rBV	1842343	2988852	14.29%	2.057%
19	10.469	1265	1272	1282	rBV	678407	1137963	5.44%	0.783%
20	10.834	1328	1334	1337	rVV	60033	96799	0.46%	0.067%
21	10.893	1339	1344	1353	rVV2	87305	156750	0.75%	0.108%
22	11.081	1370	1376	1383	rBV	308550	507809	2.43%	0.350%
23	12.581	1622	1631	1637	rBV2	136591	232004	1.11%	0.160%
24	12.957	1689	1695	1698	rBV5	39930	70212	0.34%	0.048%
25	13.104	1715	1720	1728	rVB2	421048	644580	3.08%	0.444%
26	13.304	1749	1754	1759	rBV	95585	149991	0.72%	0.103%
27	13.545	1790	1795	1801	rVB	294716	404863	1.94%	0.279%
28	13.634	1803	1810	1816	rBV	2419413	3478537	16.63%	2.394%
29	13.898	1848	1855	1860	rBV	2714333	4032801	19.28%	2.776%
30	14.075	1876	1885	1889	rBV4	118058	202542	0.97%	0.139%
31	14.210	1895	1908	1916	rVB2	2901069	6294052	30.09%	4.333%
32	14.310	1918	1925	1932	rVB2	215375	402656	1.92%	0.277%
33	14.410	1936	1942	1946	rBV	1161399	1685460	8.06%	1.160%
34	14.504	1953	1958	1963	rVB3	213759	421091	2.01%	0.290%
35	14.557	1963	1967	1974	rVB3	131903	233124	1.11%	0.160%
36	14.663	1980	1985	1989	rBV3	75139	114096	0.55%	0.079%

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Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0.1 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Title : SVOA CALIBRATION

37	14.975	2032	2038	2042	rBV2	69062	102264	0.49%	0.070%
38	15.210	2071	2078	2084	rBV	3420285	4895057	23.40%	3.370%
39	15.322	2091	2097	2105	rBV	922009	1238281	5.92%	0.852%
40	15.563	2128	2138	2143	rBV4	205195	379091	1.81%	0.261%
41	15.645	2148	2152	2155	rVV	96398	135644	0.65%	0.093%
42	15.710	2157	2163	2169	rVB	792972	1150977	5.50%	0.792%
43	15.798	2174	2178	2184	rVB7	55715	99173	0.47%	0.068%
44	16.075	2220	2225	2241	rVB3	249044	466727	2.23%	0.321%
45	16.204	2242	2247	2255	rVB2	89709	139875	0.67%	0.096%
46	16.357	2269	2273	2276	rBV2	64940	89356	0.43%	0.062%
47	16.398	2276	2280	2284	rVB	63861	82278	0.39%	0.057%
48	16.481	2290	2294	2300	rBV	44066	83255	0.40%	0.057%
49	16.892	2360	2364	2369	rBV	136298	210601	1.01%	0.145%
50	16.957	2369	2375	2386	rVB	3545491	5021305	24.01%	3.456%
51	17.057	2386	2392	2397	rBV2	3684328	5140531	24.58%	3.538%
52	17.263	2423	2427	2433	rVV2	67190	119710	0.57%	0.082%
53	17.369	2441	2445	2451	rVB3	114242	203914	0.97%	0.140%
54	17.769	2508	2513	2518	rBV3	82069	143803	0.69%	0.099%
55	17.898	2529	2535	2548	rBV	1847841	2677860	12.80%	1.843%
56	18.192	2580	2585	2591	rBV5	103772	222341	1.06%	0.153%
57	18.328	2605	2608	2613	rVB3	62056	82720	0.40%	0.057%
58	18.569	2645	2649	2651	rBV3	68826	103305	0.49%	0.071%
59	18.763	2678	2682	2686	rBV2	106794	168333	0.80%	0.116%
60	18.916	2704	2708	2713	rVB2	130914	195120	0.93%	0.134%
61	18.992	2714	2721	2724	rBV2	73985	144196	0.69%	0.099%
62	19.033	2724	2728	2730	rBV2	188590	227246	1.09%	0.156%
63	19.063	2730	2733	2740	rVV	303018	578055	2.76%	0.398%
64	19.122	2740	2743	2750	rVB	163628	202813	0.97%	0.140%
65	19.186	2750	2754	2766	rBV	1185782	1701536	8.13%	1.171%
66	19.363	2778	2784	2789	rBV	4459269	6123114	29.27%	4.215%
67	19.428	2793	2795	2798	rVV2	142035	181474	0.87%	0.125%
68	19.469	2798	2802	2808	rVB5	156249	260676	1.25%	0.179%
69	19.598	2821	2824	2828	rVB2	99612	112216	0.54%	0.077%
70	19.704	2839	2842	2847	rVB2	114610	138399	0.66%	0.095%
71	19.786	2849	2856	2860	rBV2	831586	1275161	6.10%	0.878%
72	19.828	2860	2863	2866	rVB2	73237	88850	0.42%	0.061%
73	19.933	2876	2881	2884	rBV2	876909	1089293	5.21%	0.750%
74	19.969	2884	2887	2890	rVB	218504	240851	1.15%	0.166%
75	20.222	2927	2930	2932	rBV	94776	123664	0.59%	0.085%
76	20.280	2937	2940	2944	rVV2	244284	313251	1.50%	0.216%

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 Title : SVOA CALIBRATION

77	20.339	2946	2950	2954	rVV2	229730	372742	1.78%	0.257%
78	20.375	2954	2956	2959	rVV	157374	170009	0.81%	0.117%
79	20.422	2960	2964	2970	rVV4	263771	514497	2.46%	0.354%
80	20.533	2980	2983	2987	rVB	163897	196151	0.94%	0.135%
81	20.586	2987	2992	2996	rBV	791462	930089	4.45%	0.640%
82	20.633	2998	3000	3004	rBV	133949	155429	0.74%	0.107%
83	20.745	3013	3019	3032	rVB	16642577	20917660	100.00%	14.399%
84	20.880	3037	3042	3046	rBV	1784270	2387147	11.41%	1.643%
85	20.927	3046	3050	3058	rVB	2443837	3016854	14.42%	2.077%
86	21.086	3074	3077	3081	rVB	169925	205452	0.98%	0.141%
87	21.145	3085	3087	3090	rVV2	233535	265781	1.27%	0.183%
88	21.198	3090	3096	3103	rVB	3634038	5286329	25.27%	3.639%
89	21.269	3104	3108	3114	rBV	514912	823749	3.94%	0.567%
90	21.439	3133	3137	3151	rVB4	380456	791527	3.78%	0.545%
91	22.004	3226	3233	3247	rBV	4254011	7069583	33.80%	4.866%
92	22.416	3298	3303	3309	rBV2	470221	890504	4.26%	0.613%
93	22.633	3337	3340	3356	rVB2	398336	796294	3.81%	0.548%
94	23.327	3451	3458	3461	rBV	1353455	2714896	12.98%	1.869%
95	23.363	3461	3464	3480	rVB	1257481	2583435	12.35%	1.778%
96	23.833	3536	3544	3556	rBV	2247915	5468030	26.14%	3.764%
97	24.027	3569	3577	3588	rVB2	2018015	4854377	23.21%	3.342%
98	25.151	3759	3768	3776	rBV	1842834	4907511	23.46%	3.378%
99	25.245	3777	3784	3795	rVB2	652565	1871137	8.95%	1.288%
100	28.674	4357	4367	4382	rVB5	602076	2515574	12.03%	1.732%

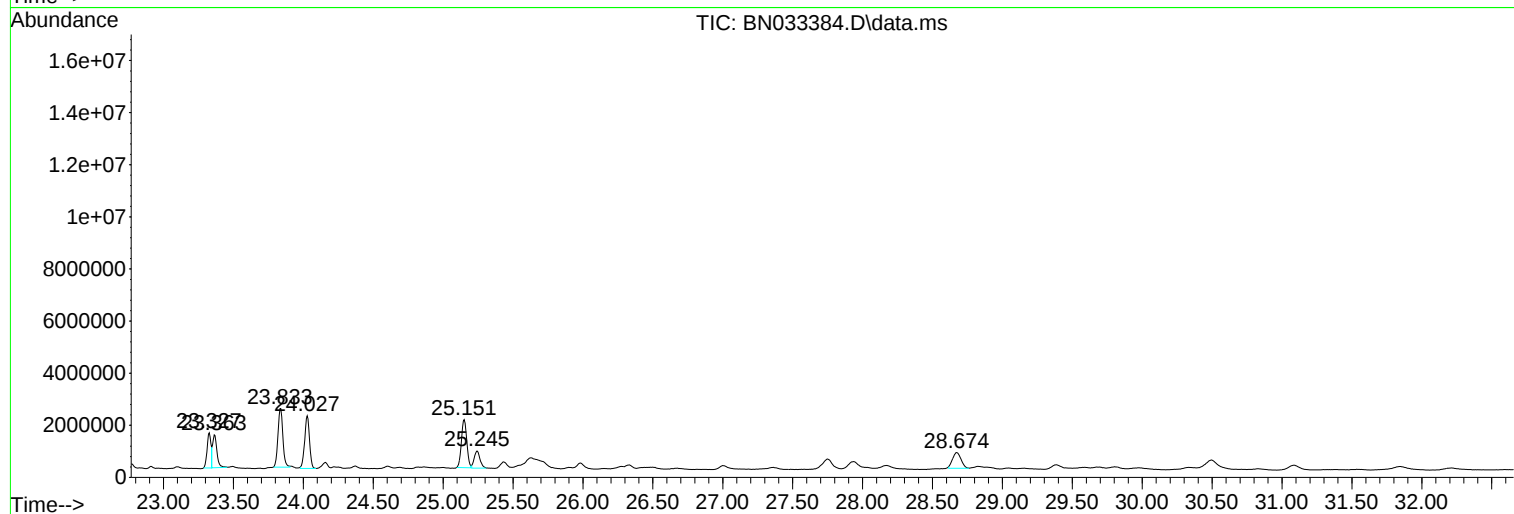
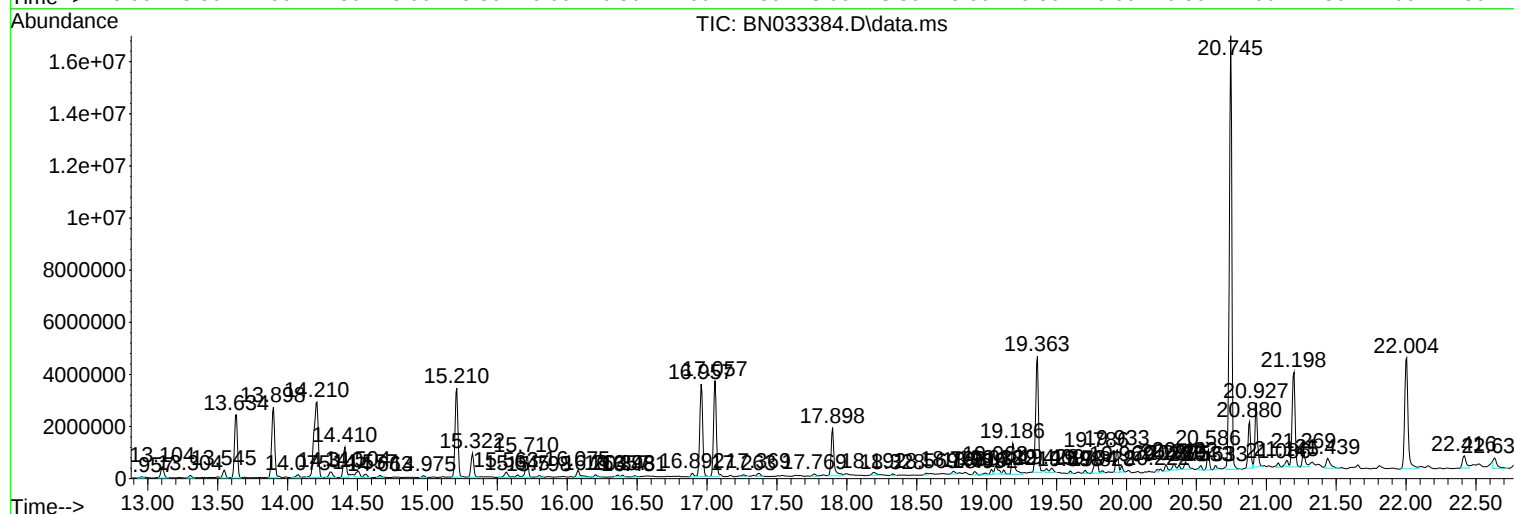
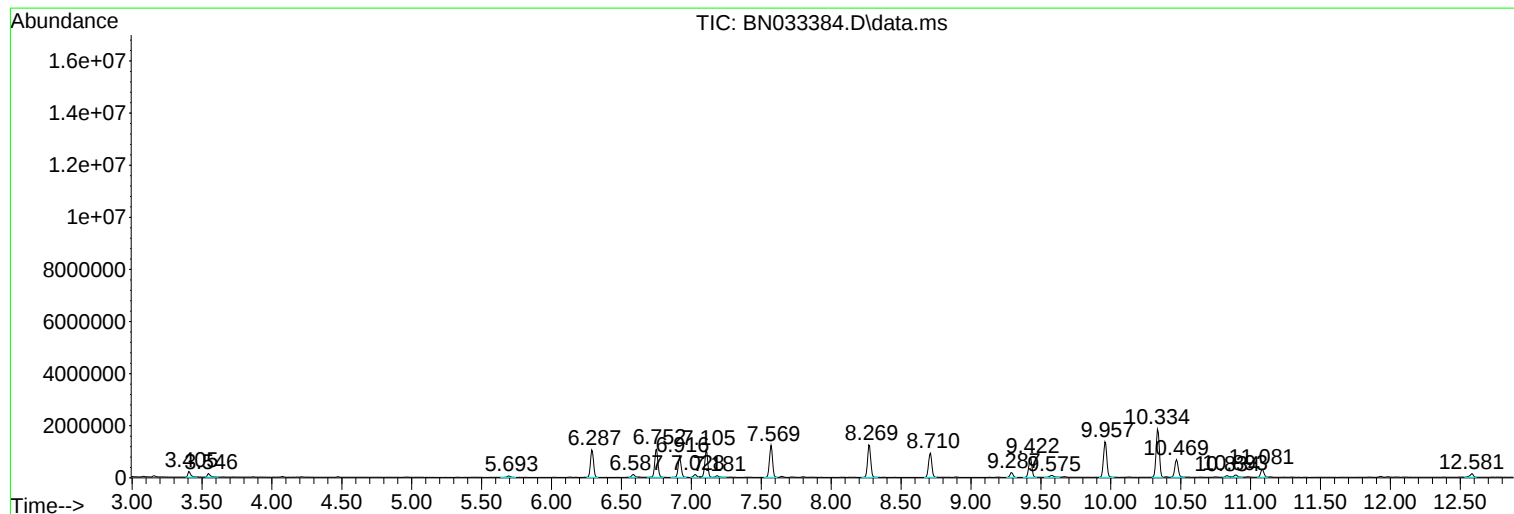
Sum of corrected areas: 145274900

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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
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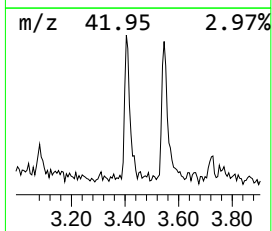
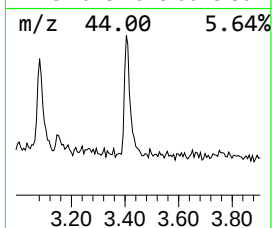
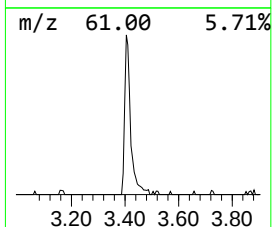
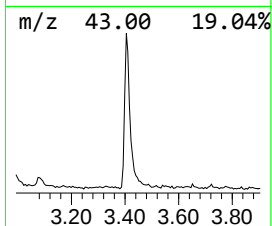
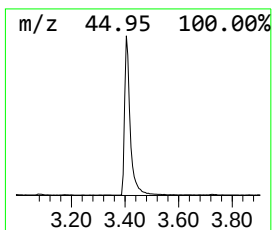
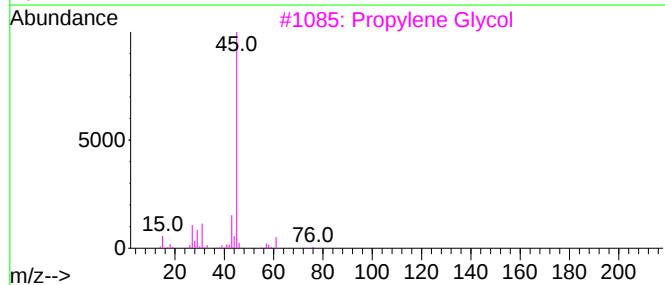
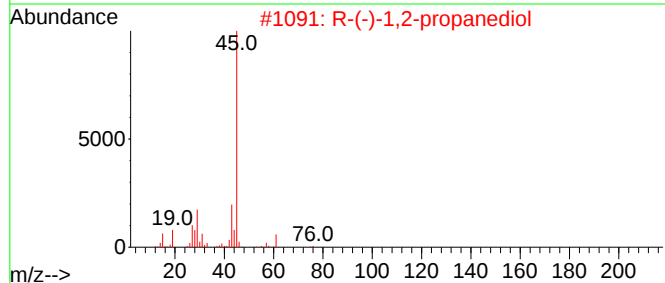
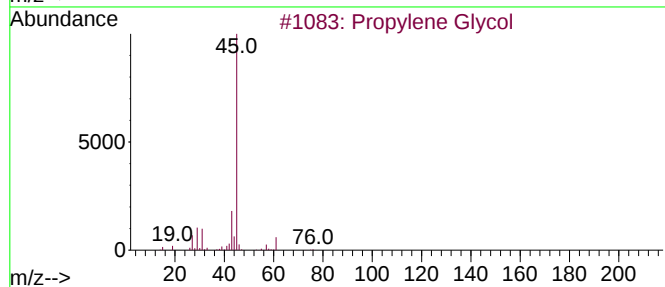
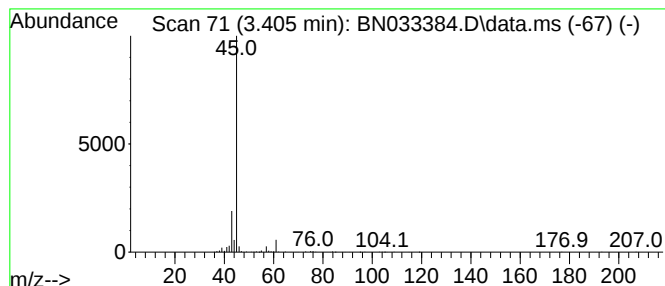
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propylene Glycol Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.405	3.36 ng/ul	314209	1,4-Dichlorobenzene-d4	7.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3			Propylene Glycol	76	C3H8O2	000057-55-6	56
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40



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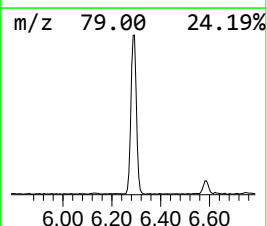
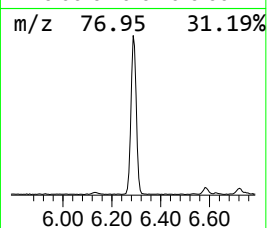
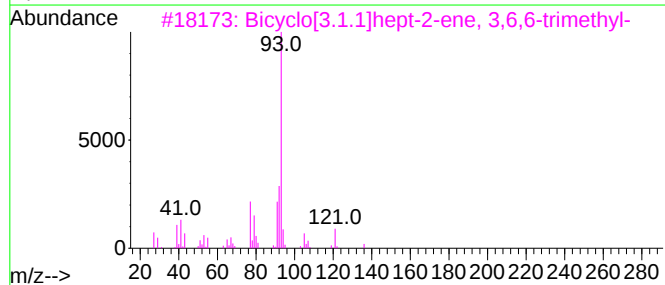
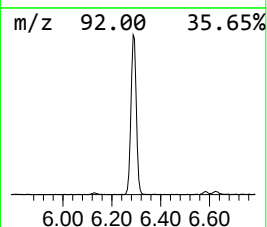
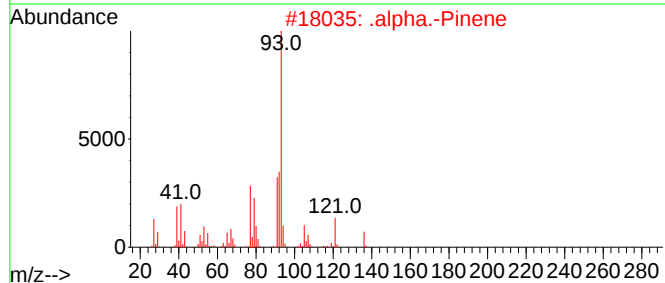
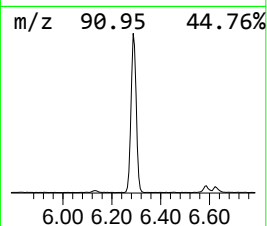
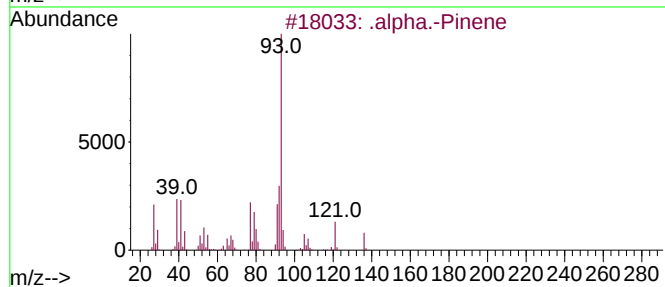
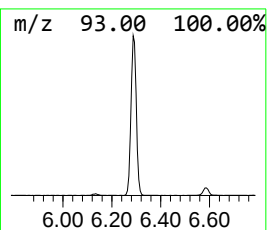
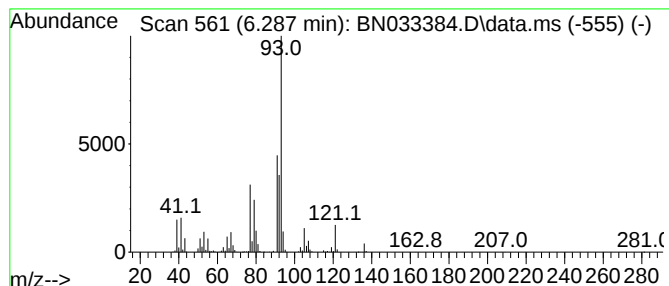
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 .alpha.-Pinene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.287	17.03 ng/ul	1591150	1,4-Dichlorobenzene-d4	7.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Pinene	136	C10H16	000080-56-8	94
2	.		.alpha.-Pinene	136	C10H16	000080-56-8	94
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...			136	C10H16	004889-83-2	91
4	(+)-3-Carene			136	C10H16	000498-15-7	91
5	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene			136	C10H16	007785-70-8	91



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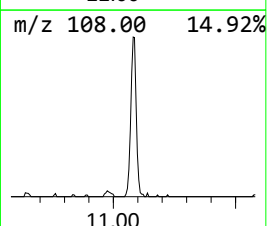
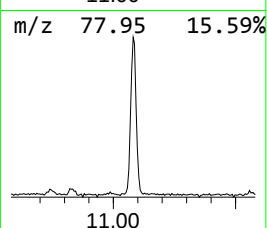
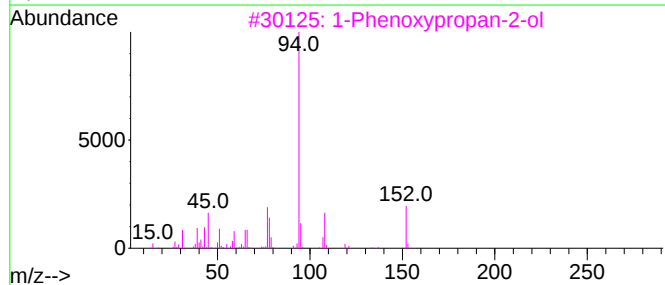
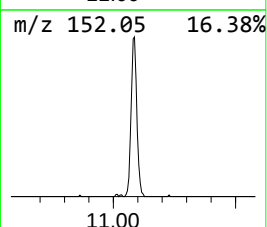
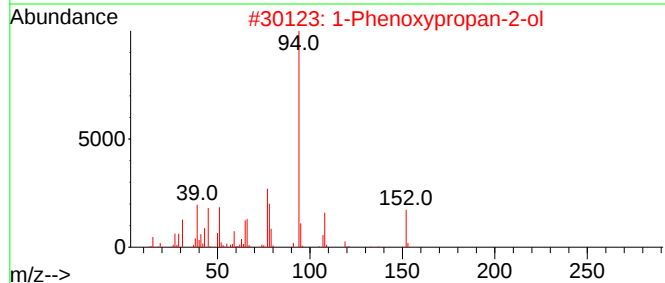
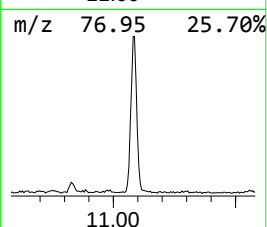
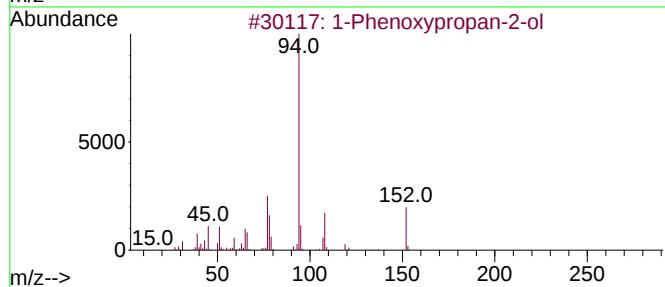
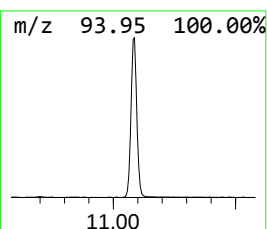
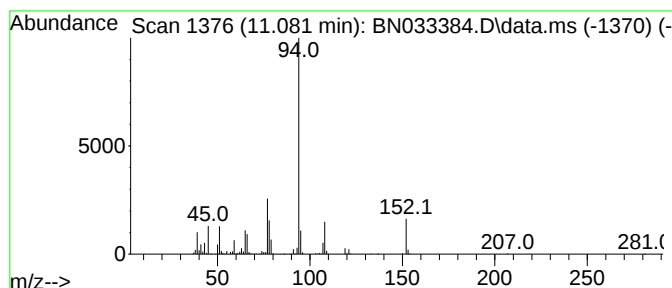
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.081	3.40 ng/ul	507809	Naphthalene-d8	10.334

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
4			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	94
5			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

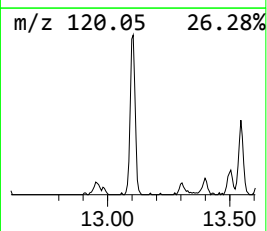
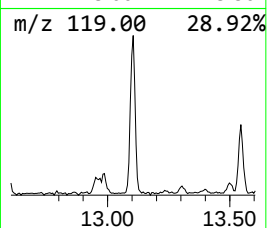
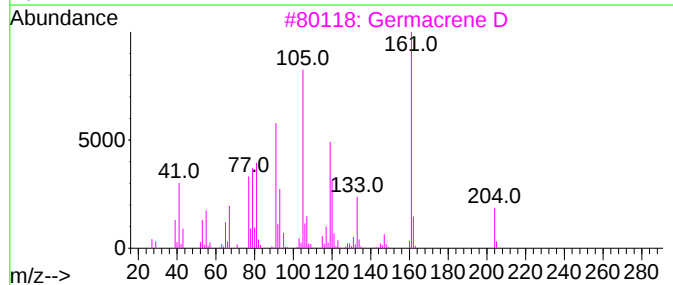
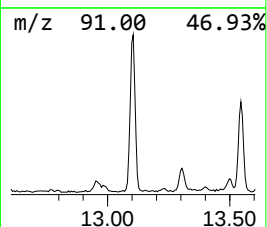
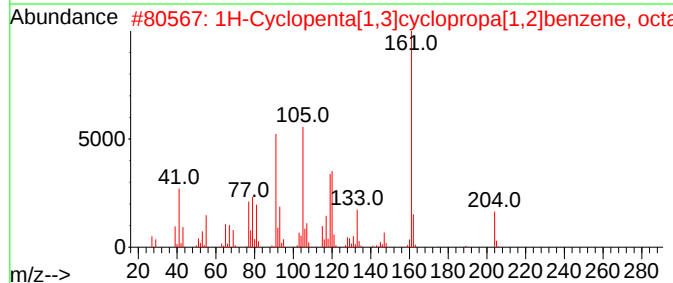
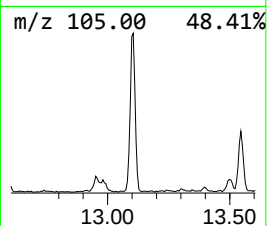
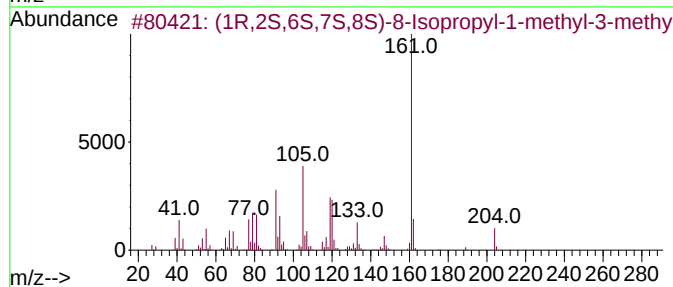
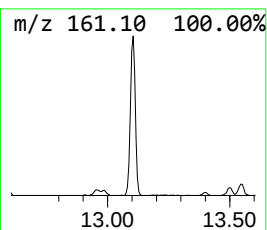
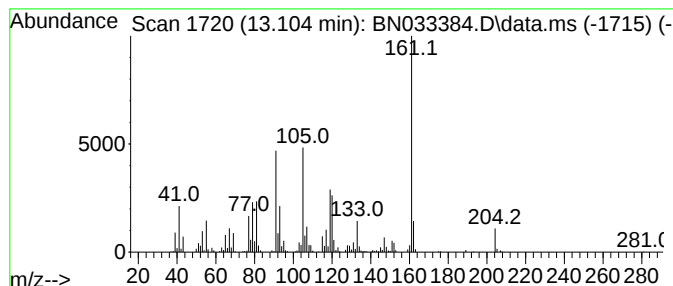
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (1R,2S,6S,7S,8S)-8-Isopropy... Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.104	2.05 ng/ul	644580	Acenaphthene-d10	14.210	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	99
2	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	98
3	Germacrene D	204	C15H24	023986-74-5	98
4	Germacrene D	204	C15H24	023986-74-5	96
5	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
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Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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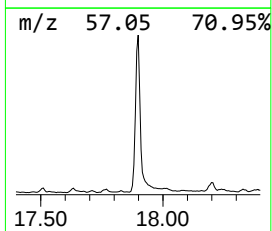
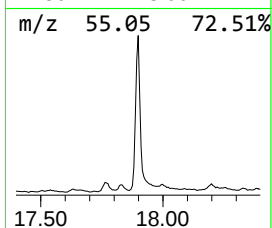
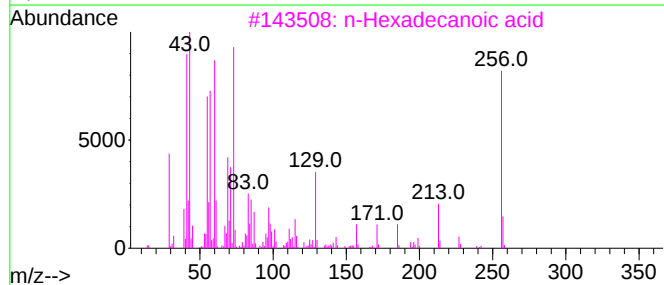
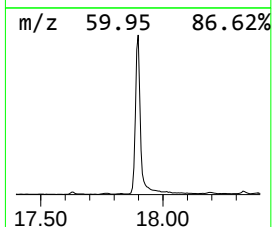
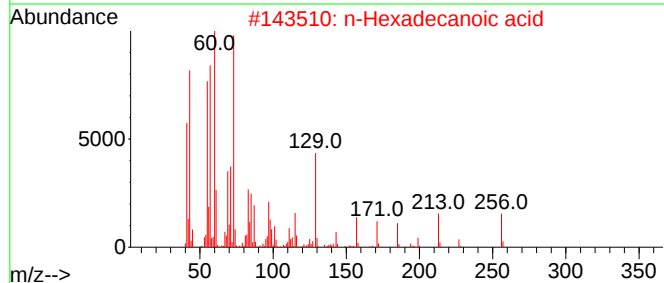
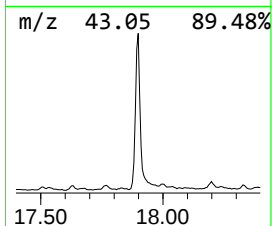
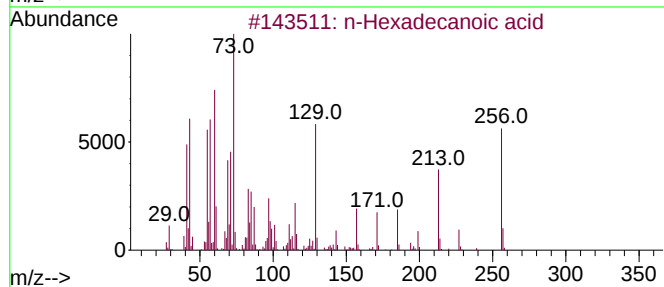
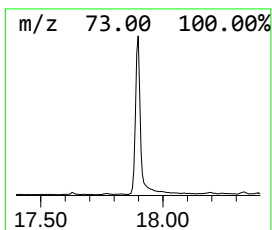
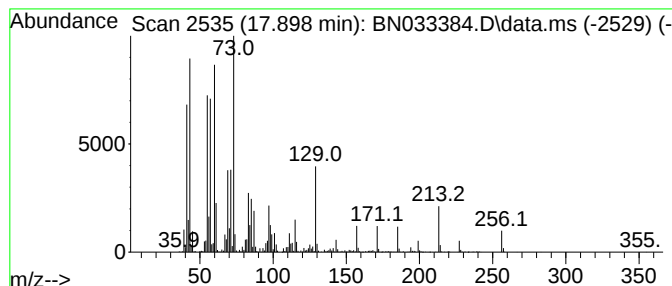
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.898	10.67 ng/ul	2677860	Phenanthrene-d10	16.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
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Operator : MA/JU
Sample : P3502-21
Misc :
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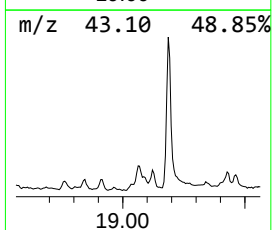
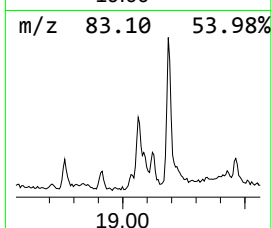
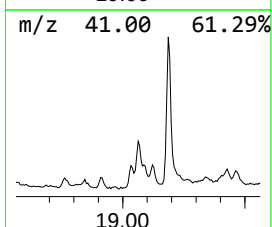
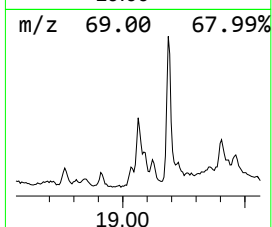
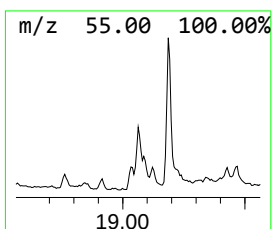
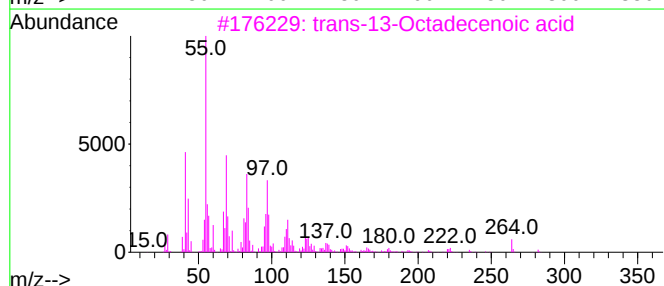
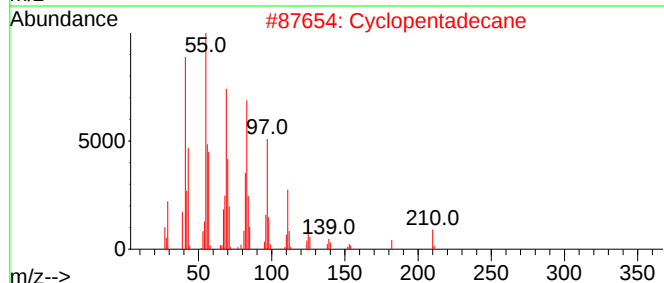
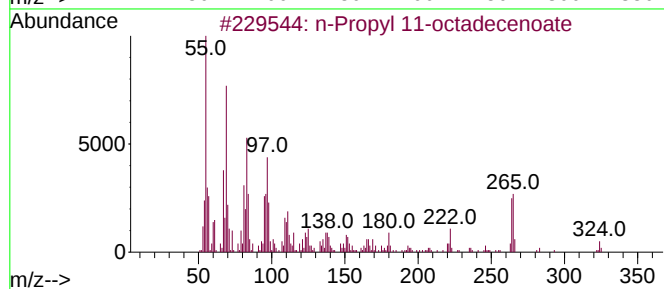
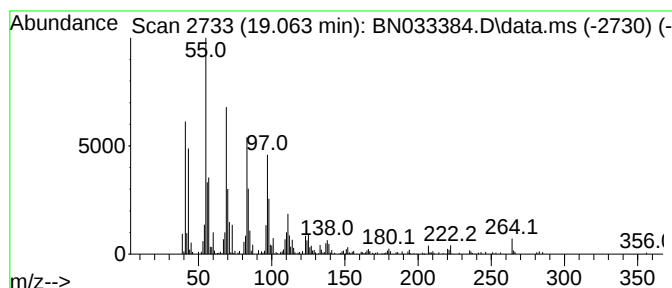
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Propyl 11-octadecenoate Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.063	2.30 ng/ul	578055	Phenanthrene-d10		16.957	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Propyl 11-octadecenoate		324	C21H40O2	1000336-71-7	91
2	Cyclopentadecane		210	C15H30	000295-48-7	86
3	trans-13-Octadecenoic acid		282	C18H34O2	000693-71-0	83
4	9-Octadecenoic acid, (E)-		282	C18H34O2	000112-79-8	78
5	Cyclopentadecane		210	C15H30	000295-48-7	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
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Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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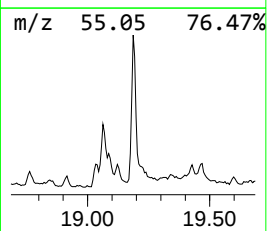
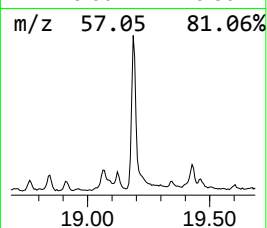
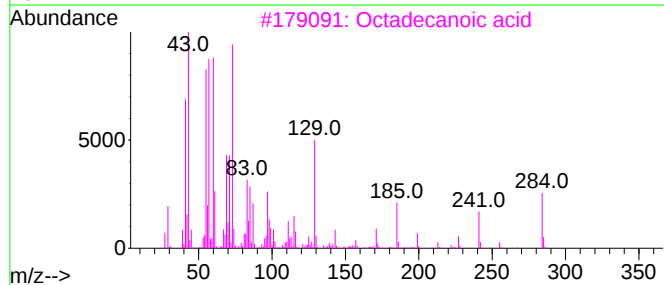
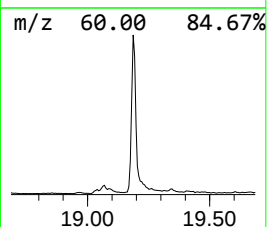
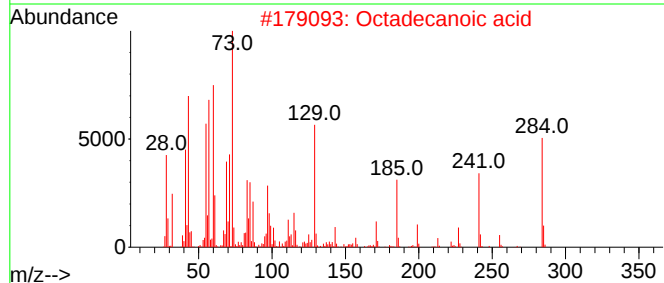
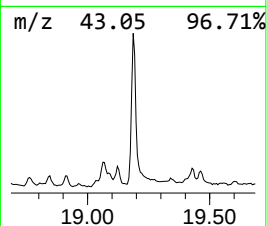
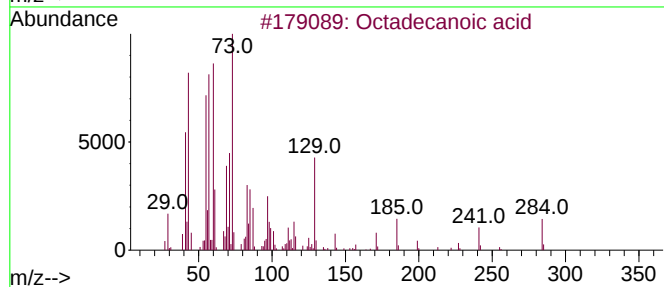
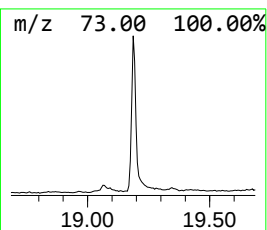
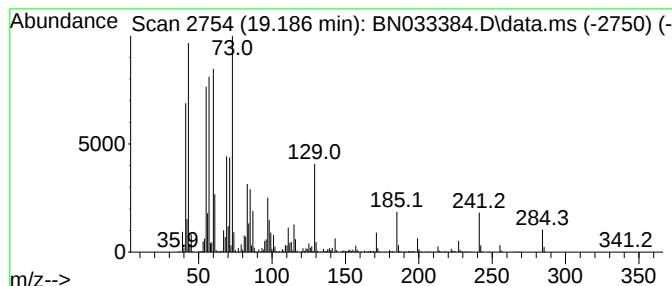
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.186	6.44 ng/ul	1701540	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	99
3			Octadecanoic acid	284	C18H36O2	000057-11-4	99
4			Octadecanoic acid	284	C18H36O2	000057-11-4	96
5			Octadecanoic acid	284	C18H36O2	000057-11-4	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

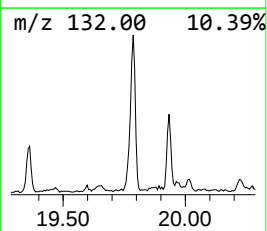
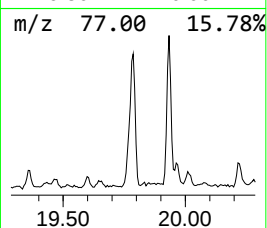
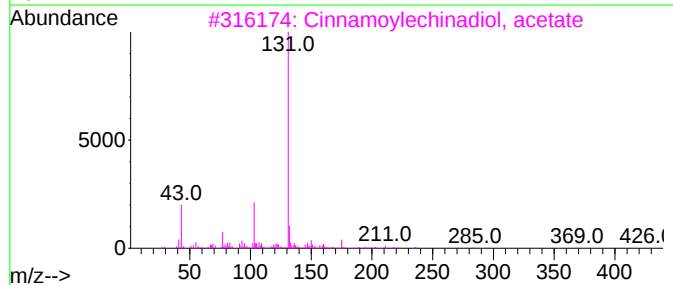
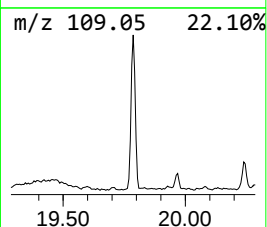
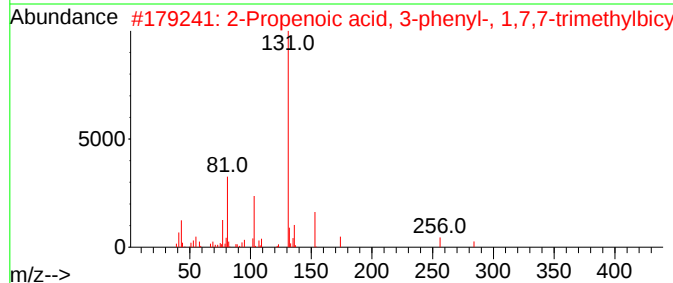
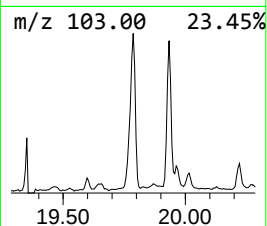
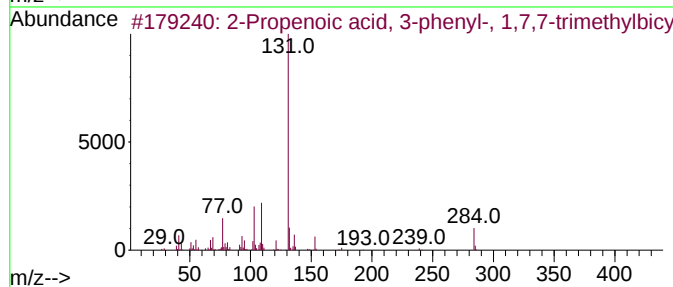
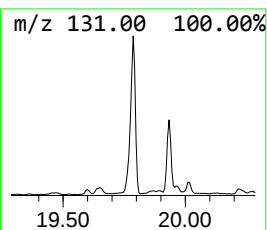
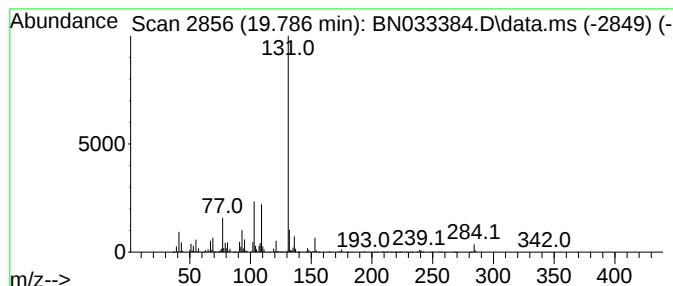
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 2-Propenoic acid, 3-phenyl-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.786	4.82 ng/ul	1275160	Chrysene-d12	21.198	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 3-phenyl-, 1,7...	284	C19H24O2	006330-67-2	98
2	2-Propenoic acid, 3-phenyl-, 1,7...	284	C19H24O2	006330-67-2	59
3	Cinnamoylchirinadiol, acetate	426	C26H34O5	1000503-42-5	53
4	1-(4-Ethynylphenyl)-2-methylprop...	174	C12H14O	1000466-39-4	53
5	N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
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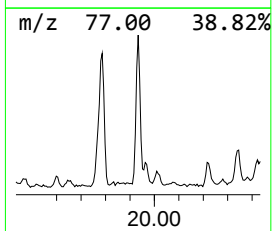
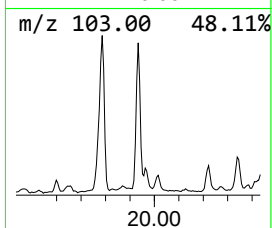
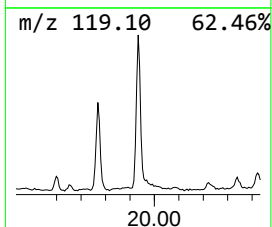
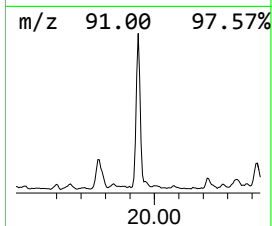
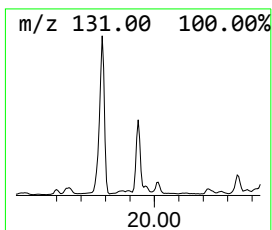
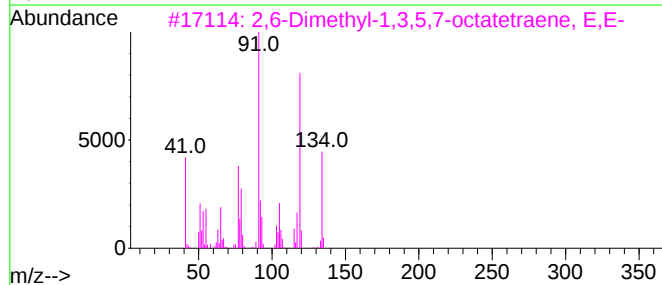
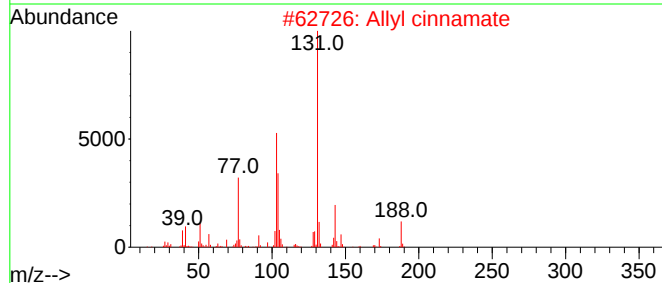
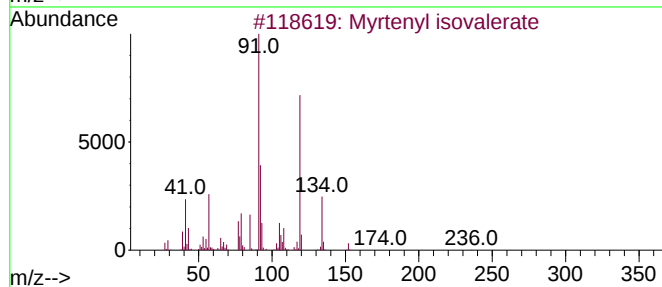
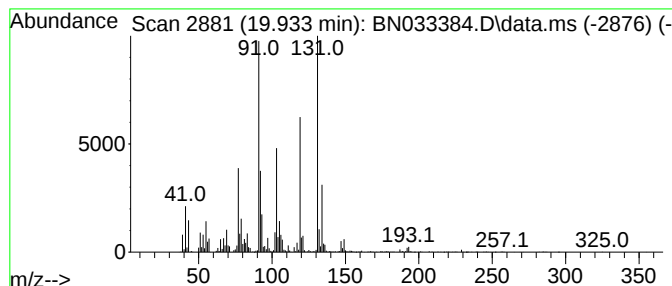
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Myrtenyl isovalerate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.933	4.12 ng/ul	1089290	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Myrtenyl isovalerate	236	C15H24O2	033900-84-4	51
2			Allyl cinnamate	188	C12H12O2	001866-31-5	47
3			2,6-Dimethyl-1,3,5,7-octatetraen...	134	C10H14	000460-01-5	46
4			3-phenylprop-2-enoic anhydride	278	C18H14O3	1010401-87-5	43
5			trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
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Misc :
ALS Vial : 12 Sample Multiplier: 1

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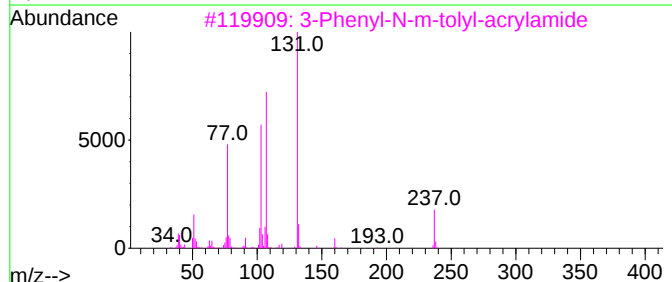
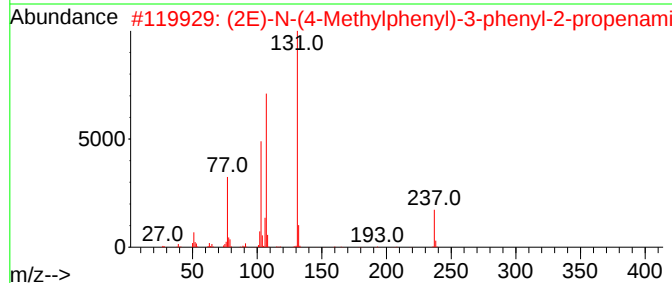
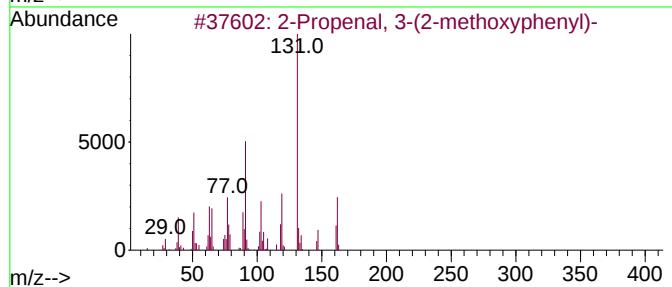
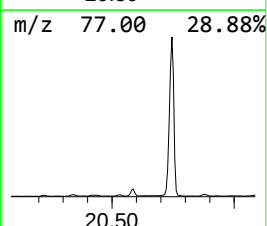
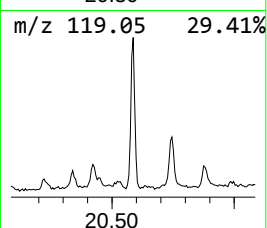
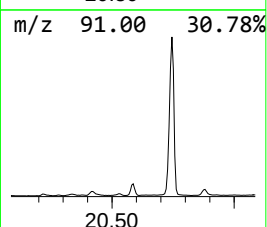
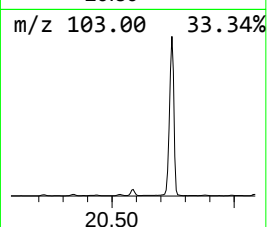
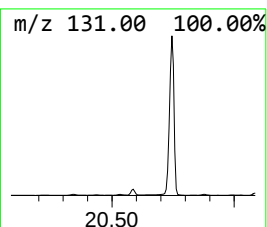
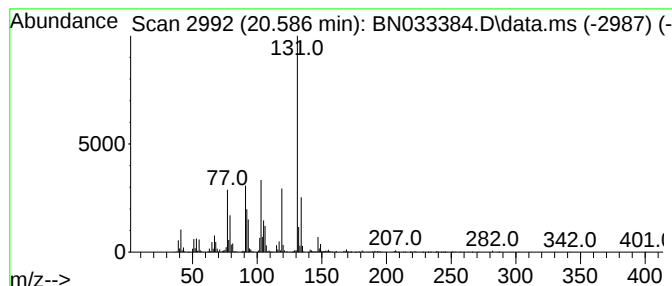
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2-Propenal, 3-(2-methoxyphene... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.586	3.52 ng/ul	930089	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propenal, 3-(2-methoxyphenyl)-	162	C10H10O2	001504-74-1	53
2			(2E)-N-(4-Methylphenyl)-3-phenyl...	237	C16H15NO	134430-88-9	50
3			3-Phenyl-N-m-tolyl-acrylamide	237	C16H15NO	1000296-12-9	47
4			(Z)-2-Methoxycinnamaldehyde	162	C10H10O2	076760-43-5	47
5			1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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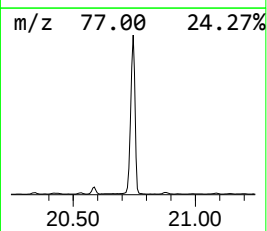
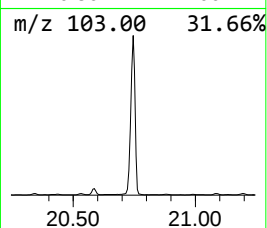
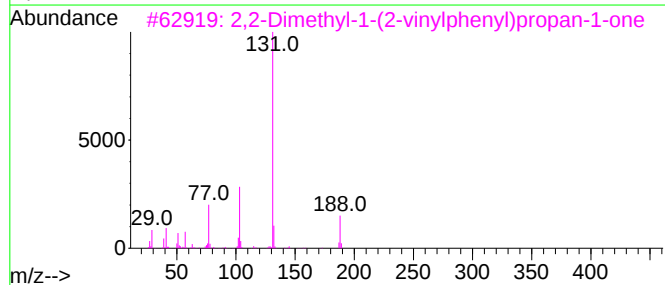
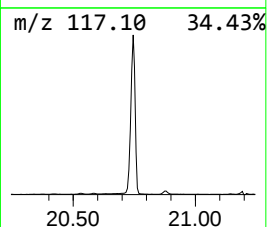
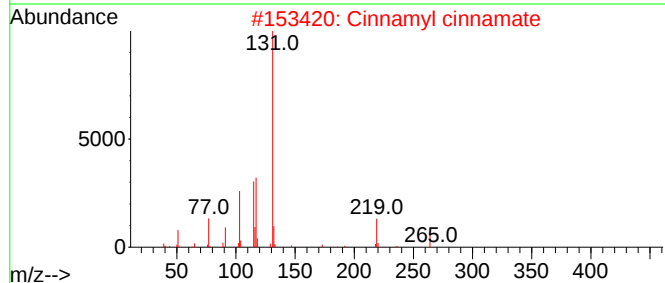
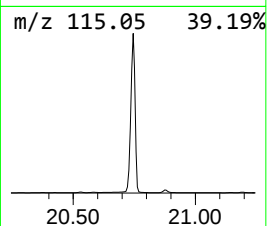
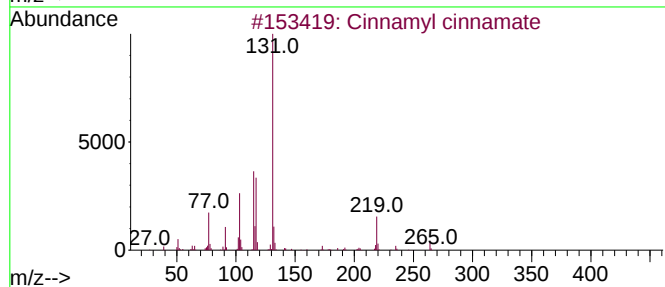
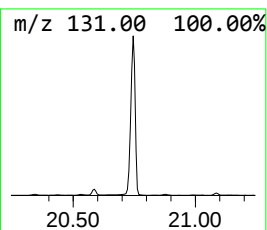
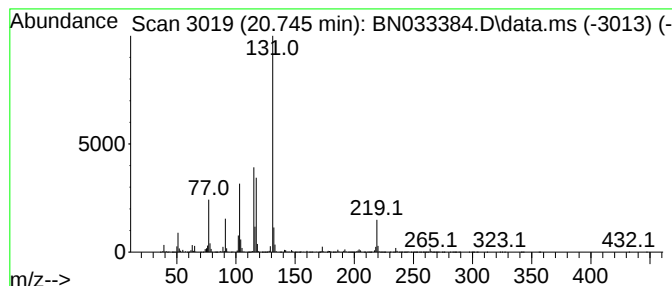
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.745	79.14 ng/ul	20917700	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
3			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	49
4			(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	49
5			N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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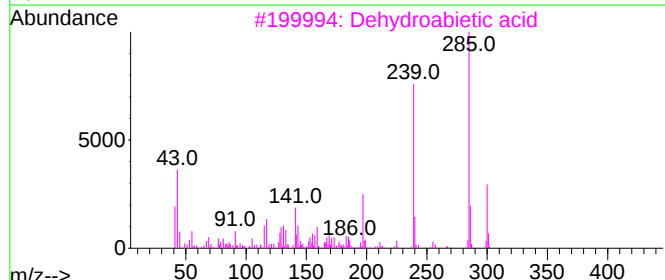
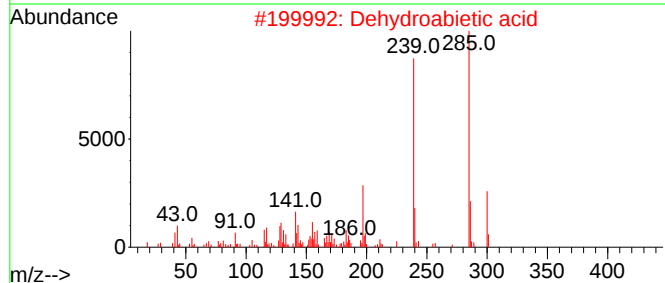
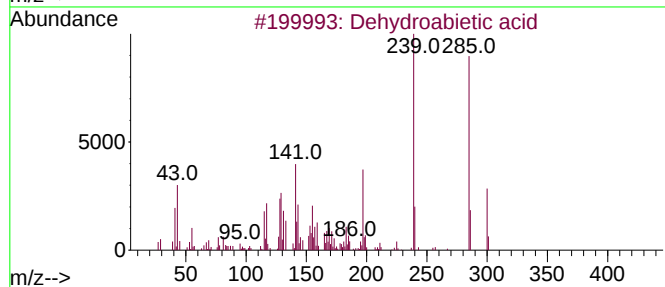
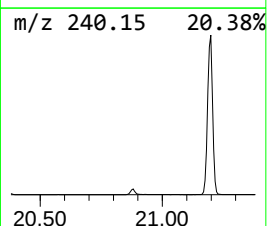
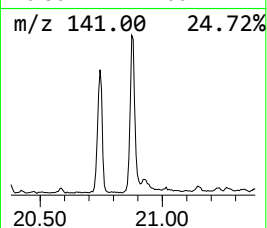
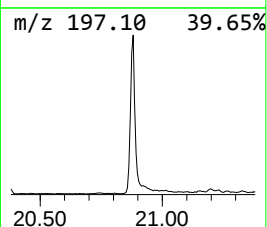
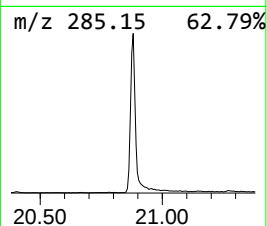
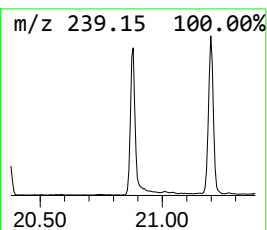
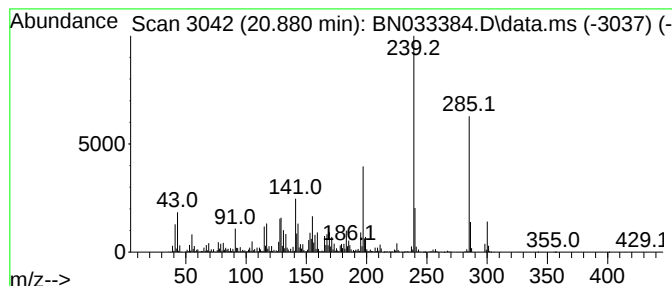
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Dehydroabiatic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.880	9.03 ng/ul	2387150	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dehydroabiatic acid	300	C20H28O2	001740-19-8	99
2			Dehydroabiatic acid	300	C20H28O2	001740-19-8	98
3			Dehydroabiatic acid	300	C20H28O2	001740-19-8	93
4			Dehydroabiatic acid	300	C20H28O2	001740-19-8	90
5			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
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Sample : P3502-21
Misc :
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Instrument :
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ClientSampleId :
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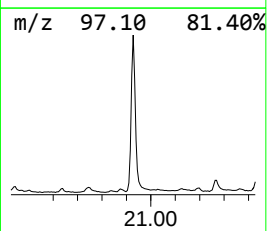
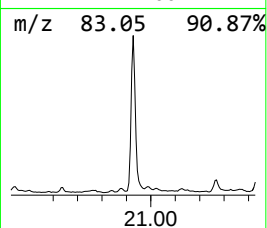
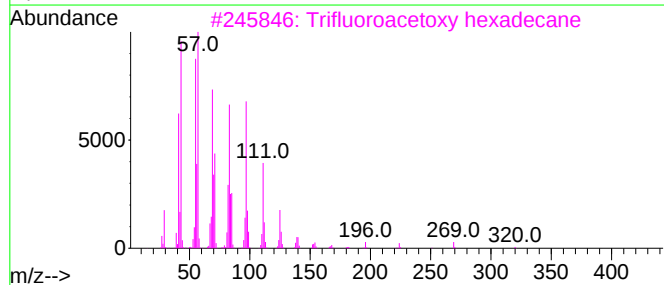
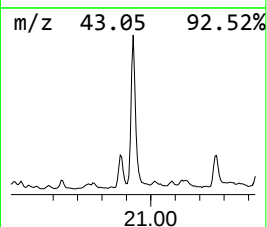
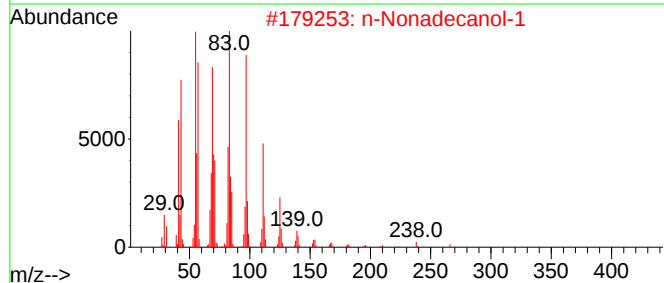
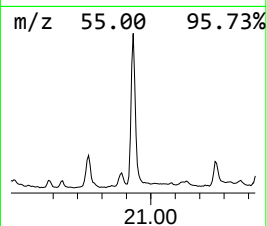
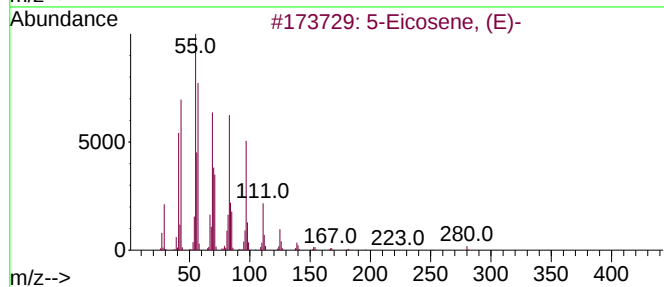
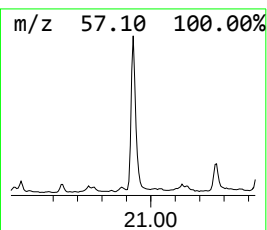
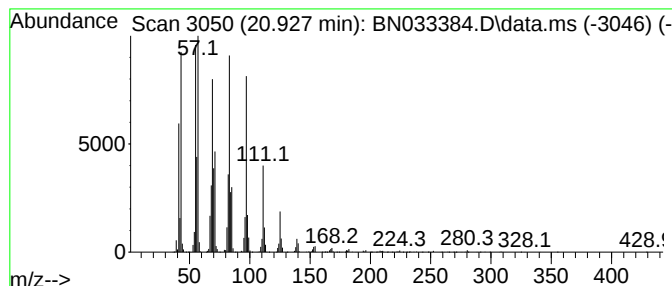
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.927	11.41 ng/ul	3016850	Chrysene-d12	21.198

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	99
2	n-Nonadecanol-1		284	C19H40O	001454-84-8	95
3	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	94
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
5	1-Heneicosanol		312	C21H44O	015594-90-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
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Misc :
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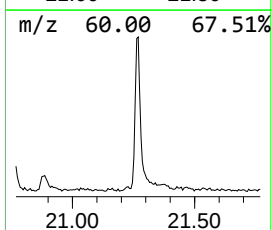
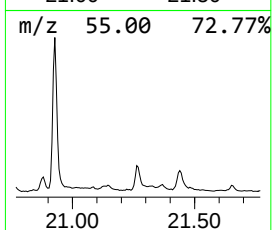
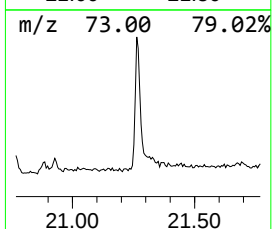
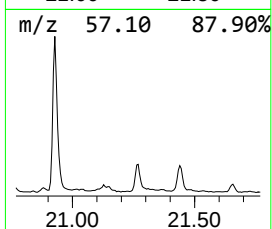
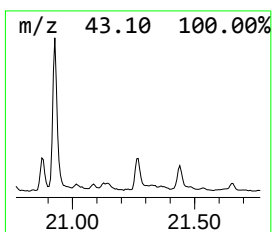
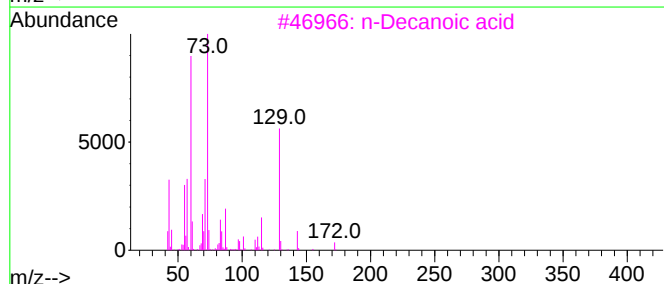
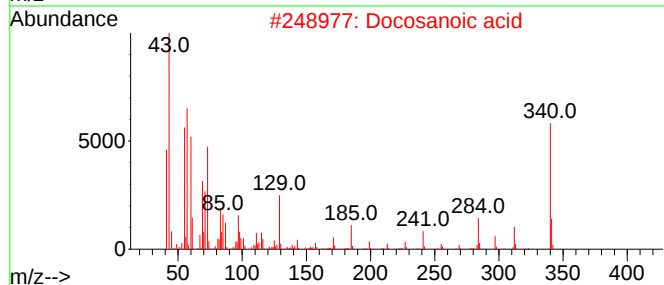
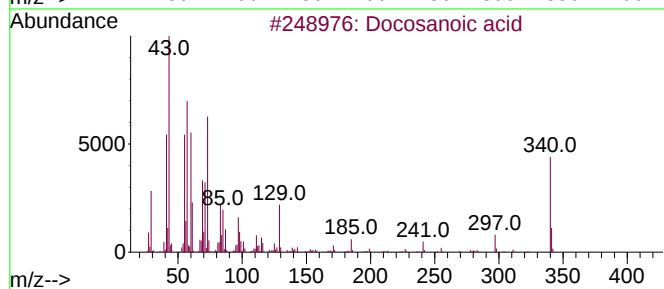
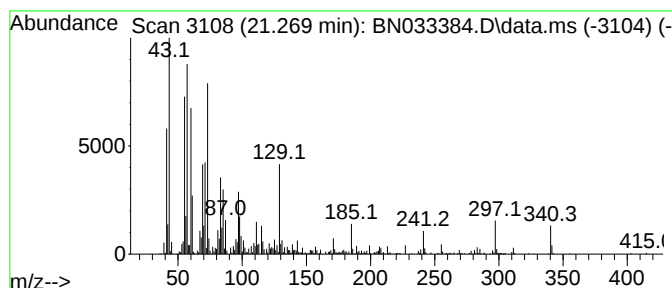
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Docosanoic acid Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.269	3.12 ng/ul	823749	Chrysene-d12	21.198	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid	340	C22H44O2	000112-85-6	96
2	Docosanoic acid	340	C22H44O2	000112-85-6	90
3	n-Decanoic acid	172	C10H20O2	000334-48-5	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Docosanoic acid	340	C22H44O2	000112-85-6	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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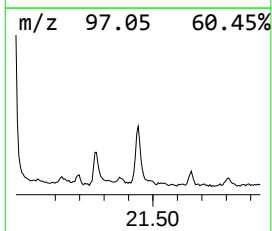
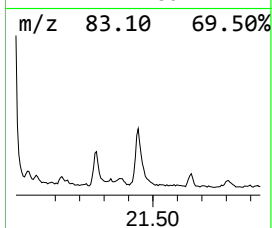
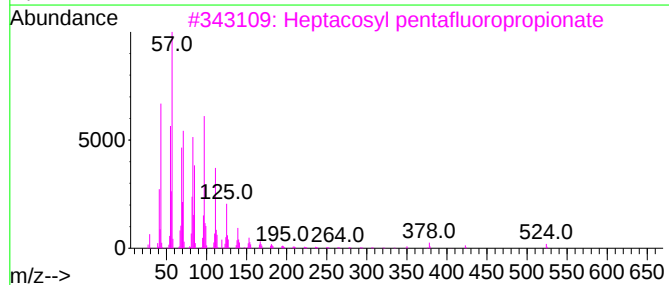
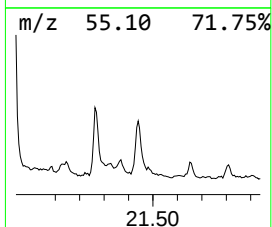
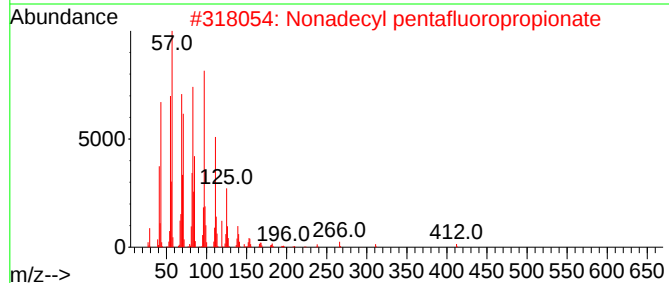
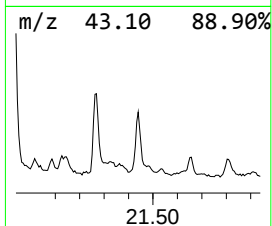
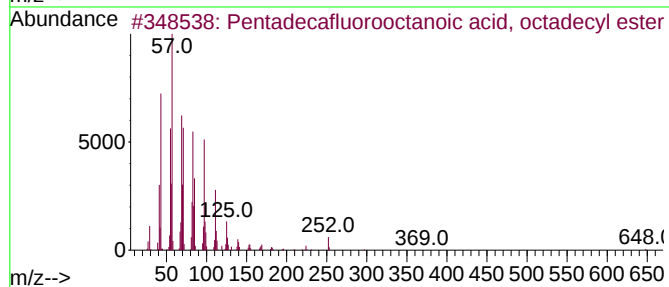
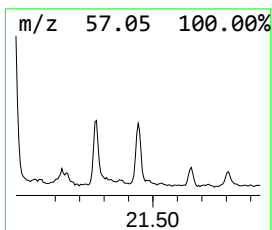
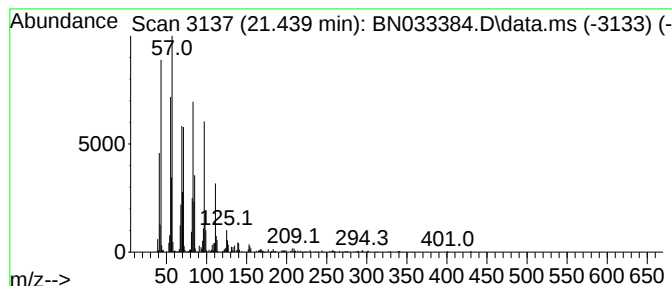
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Pentadecafluorooctanoic aci... Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.439	2.99 ng/ul	791527	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3			Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	83
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	83
5			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
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Operator : MA/JU
Sample : P3502-21
Misc :
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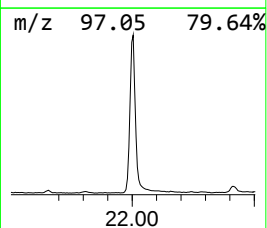
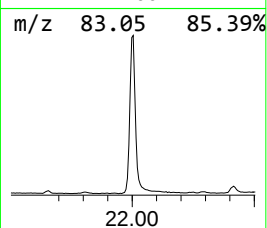
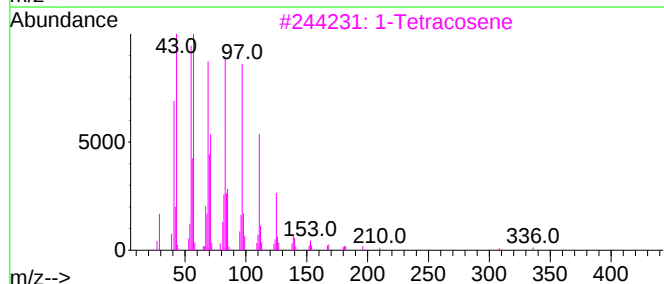
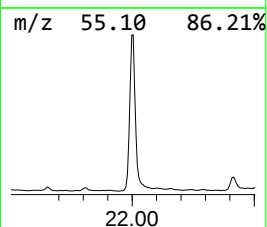
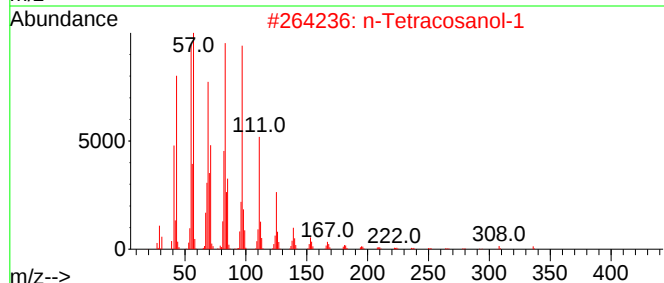
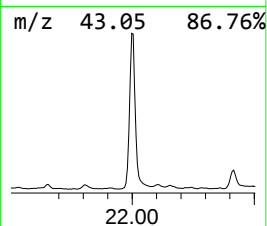
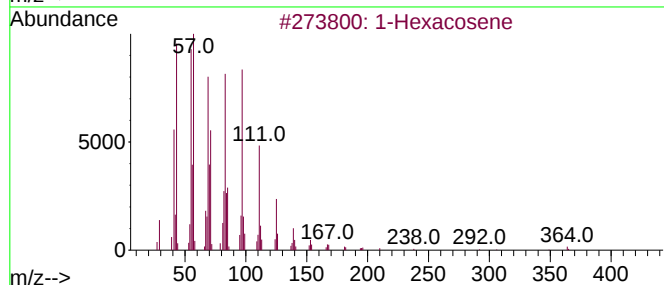
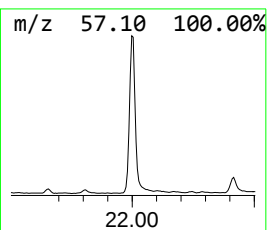
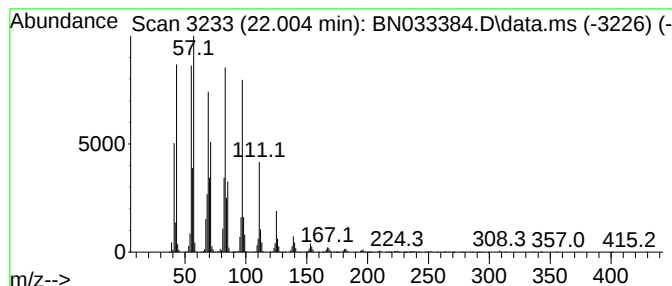
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.004	26.75 ng/ul	7069580	Chrysene-d12		21.198	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Hexacosene		364	C26H52	018835-33-1	95
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
3	1-Tetracosene		336	C24H48	010192-32-2	94
4	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
5	1-Heneicosyl formate		340	C22H44O2	077899-03-7	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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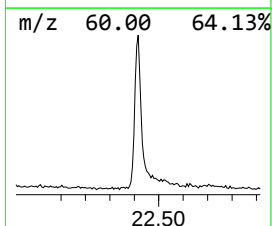
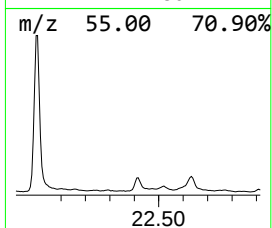
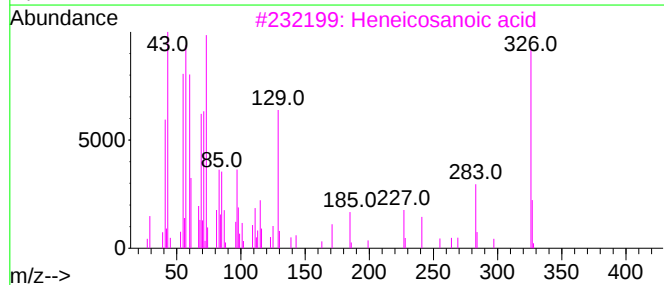
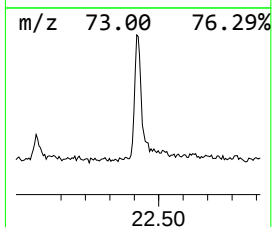
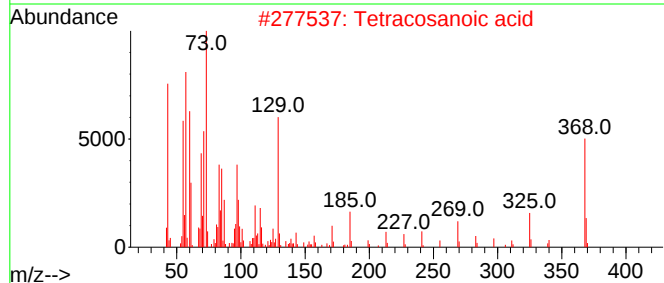
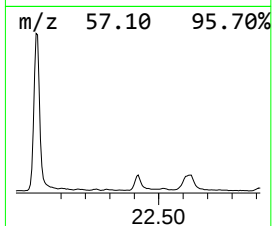
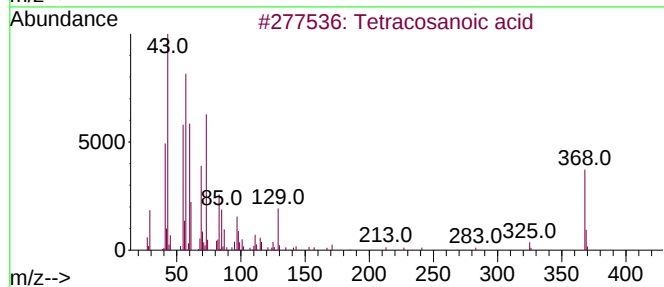
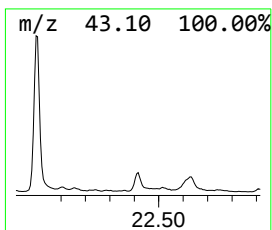
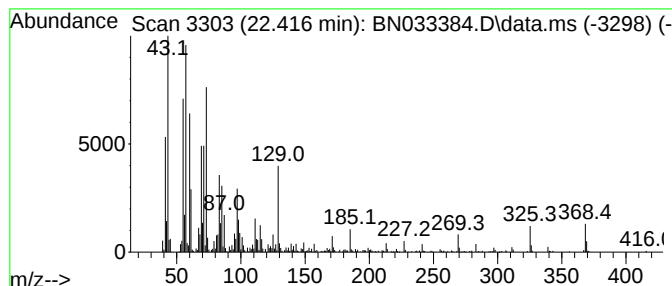
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Tetracosanoic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.416	3.37 ng/ul	890504	Chrysene-d12	21.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosanoic acid	368	C24H48O2	000557-59-5	99
2			Tetracosanoic acid	368	C24H48O2	000557-59-5	99
3			Heneicosanoic acid	326	C21H42O2	002363-71-5	98
4			Tetracosanoic acid	368	C24H48O2	000557-59-5	96
5			Octadecanoic acid	284	C18H36O2	000057-11-4	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
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Acq On : 14 Aug 2024 15:57
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Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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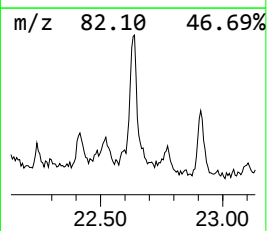
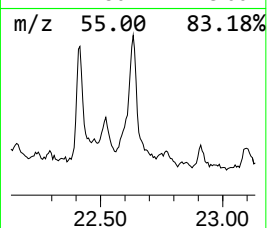
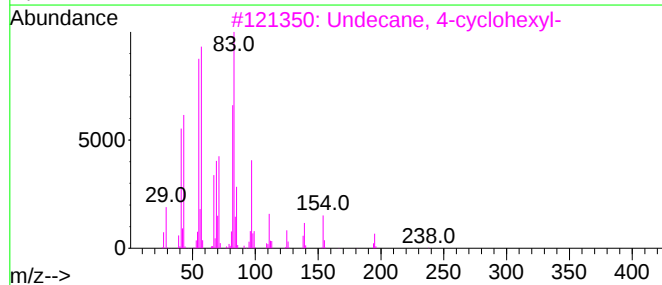
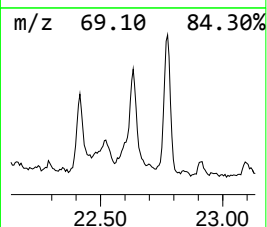
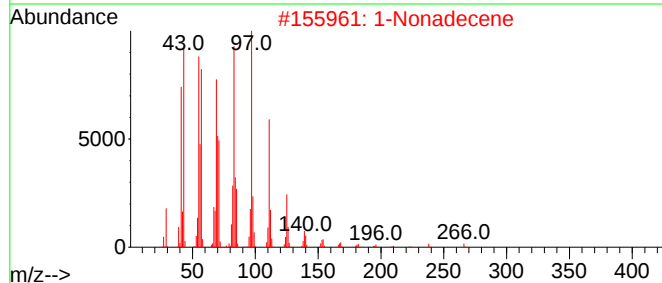
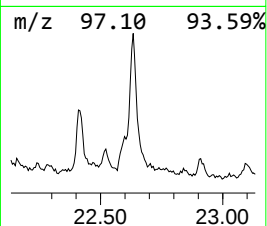
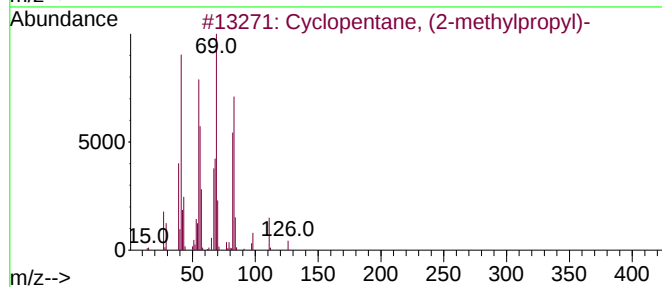
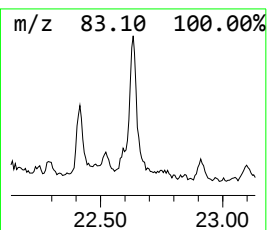
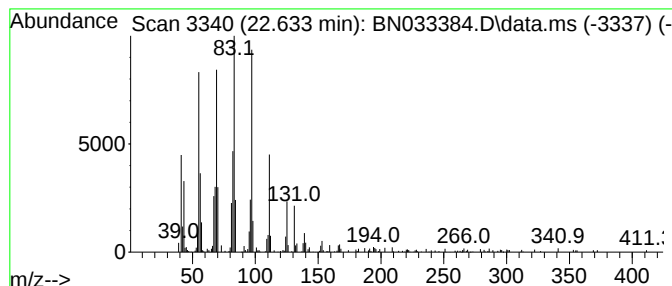
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 (DEL) Alkane: Cyclic22.633 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.633	3.28 ng/ul	796294	Perylene-d12	24.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	38
2		1-Nonadecene	266	C19H38	018435-45-5	38
3		Undecane, 4-cyclohexyl-	238	C17H34	013151-79-6	30
4		10-Heneicosene (c,t)	294	C21H42	095008-11-0	27
5		1H-Pyrazole-1-carboxaldehyde, 4-...	168	C9H16N2O	054411-09-5	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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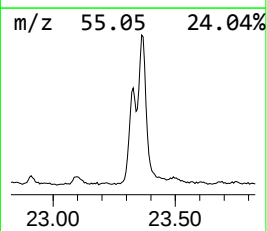
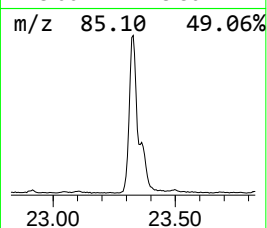
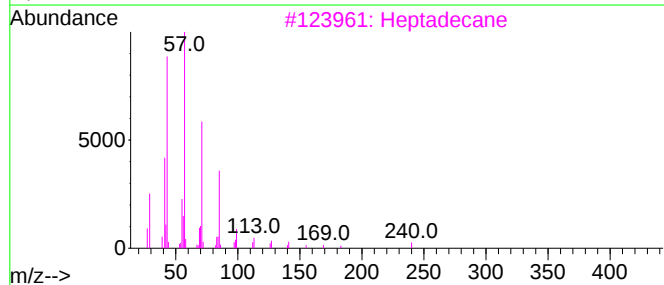
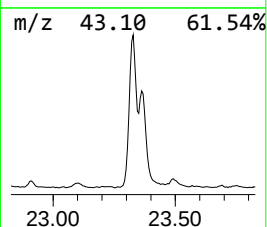
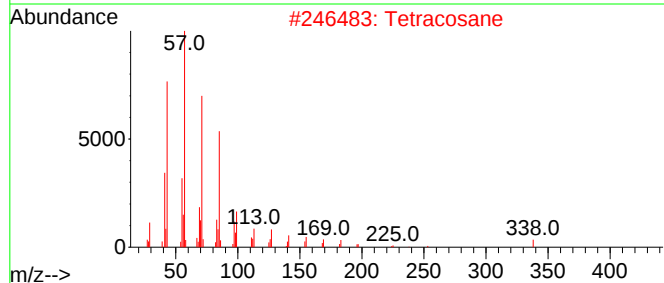
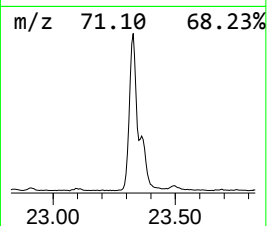
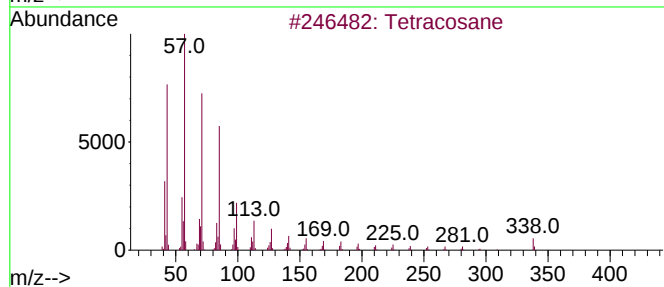
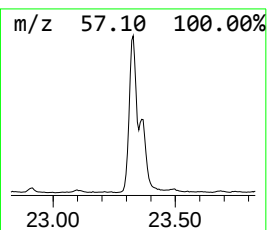
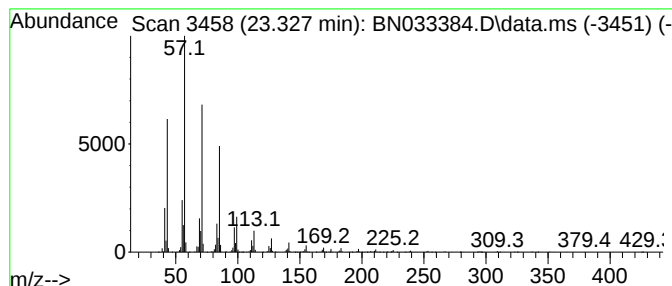
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.327	11.19 ng/ul	2714900	Perylene-d12	24.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	96
2			Tetracosane	338	C24H50	000646-31-1	94
3			Heptadecane	240	C17H36	000629-78-7	94
4			Octacosane	394	C28H58	000630-02-4	91
5			Eicosane, 3-methyl-	296	C21H44	006418-46-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
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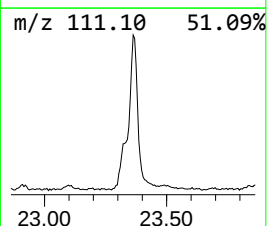
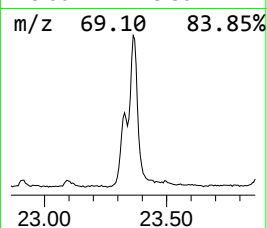
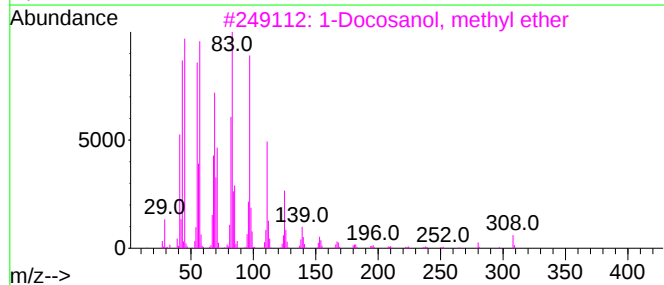
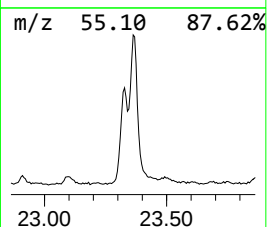
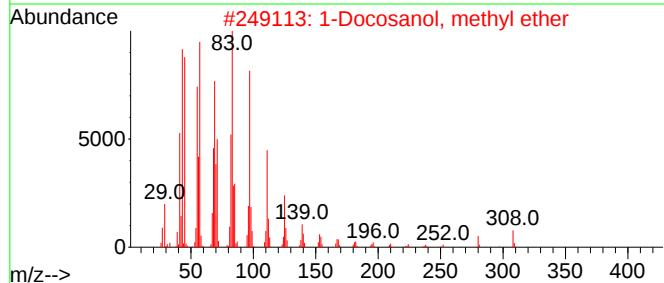
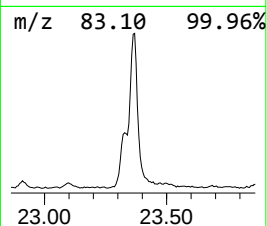
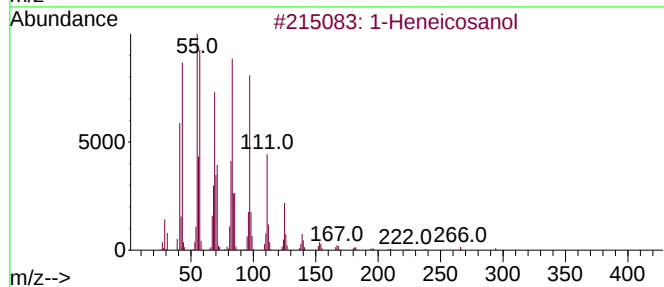
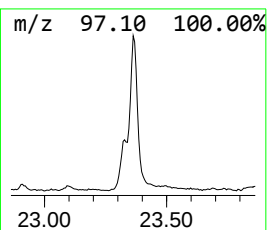
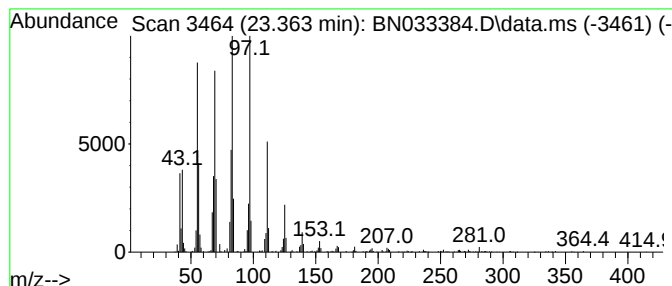
Instrument :
BNA_N
ClientSampleId :
DCXV5

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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 21 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.363	10.64 ng/ul	2583440	Perylene-d12		24.027	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	87
2	1-Docosanol, methyl ether		340	C23H48O	1000333-91-9	83
3	1-Docosanol, methyl ether		340	C23H48O	1000333-91-9	81
4	n-Heptadecanol-1		256	C17H36O	001454-85-9	72
5	1-Octadecanol		270	C18H38O	000112-92-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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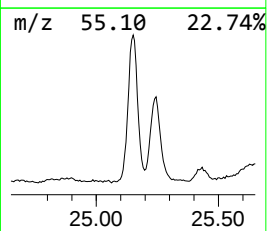
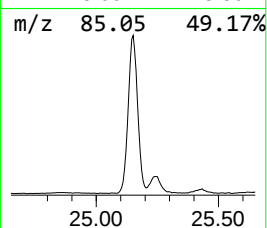
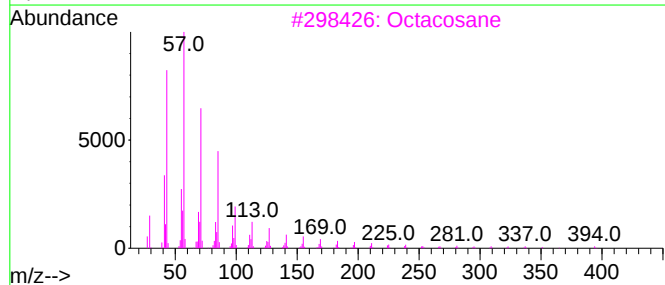
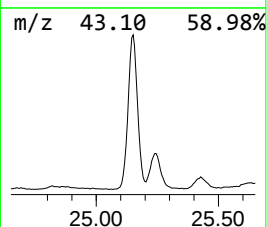
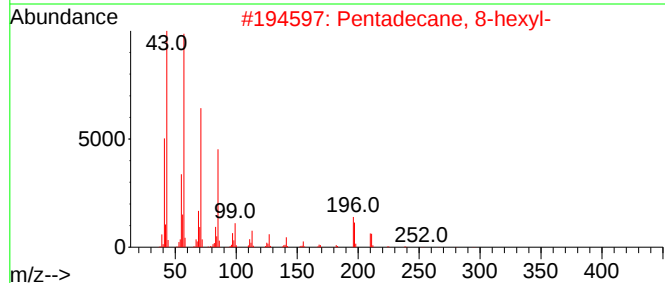
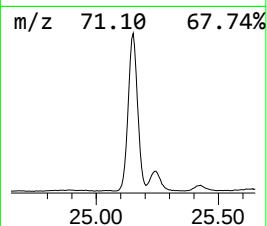
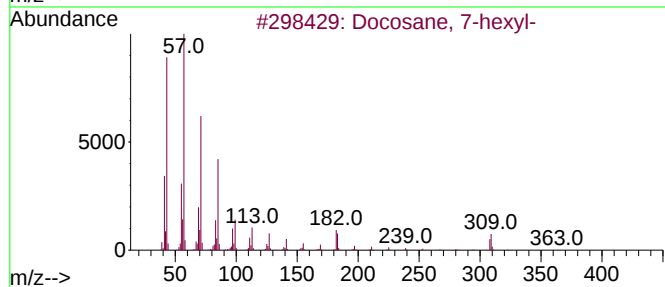
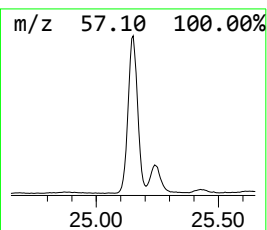
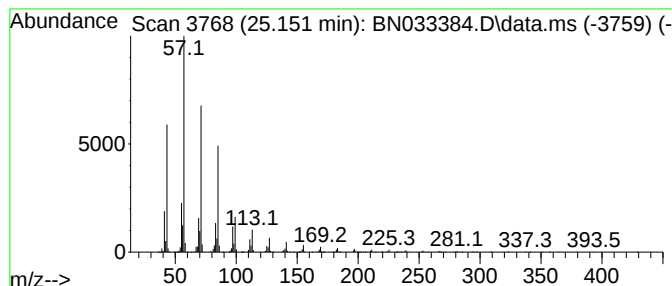
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 22 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.151	20.22 ng/ul	4907510	Perylene-d12	24.027

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosane, 7-hexyl-	394	C28H58	055373-86-9	95
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3		Octacosane	394	C28H58	000630-02-4	91
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5		Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
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Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

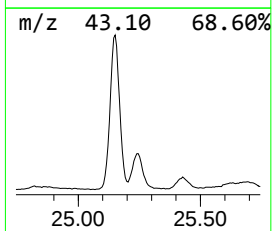
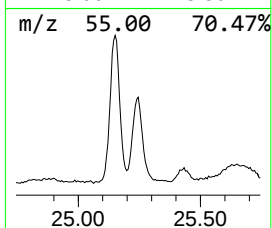
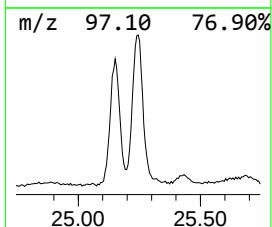
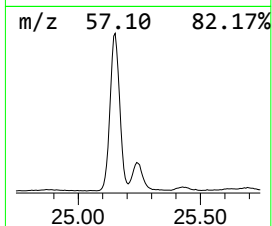
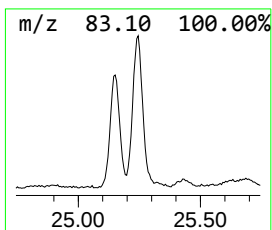
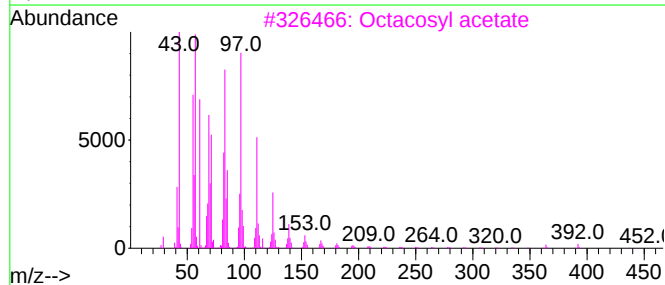
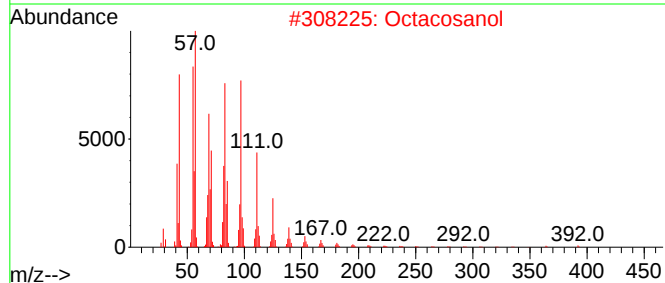
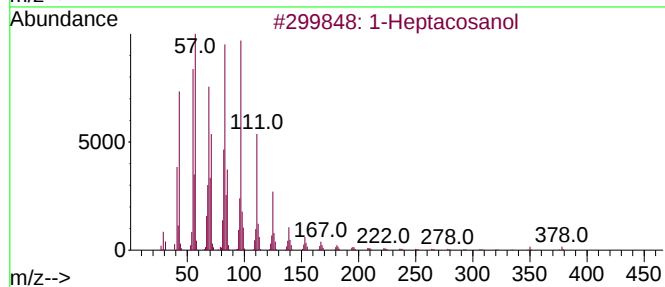
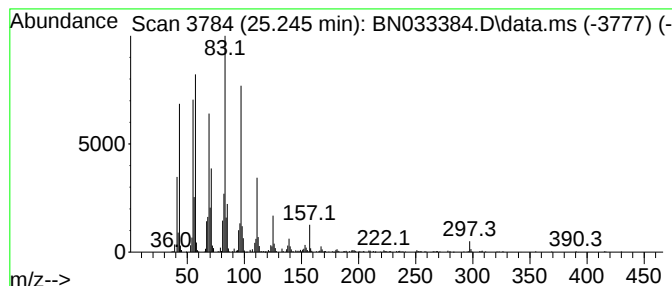
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 23 1-Heptacosanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.245	7.71 ng/ul	1871140	Perylene-d12	24.027	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	Octacosanol	410	C28H58O	000557-61-9	91
3	Octacosyl acetate	452	C30H60O2	018206-97-8	64
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	64
5	1-Hexacosene	364	C26H52	018835-33-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
Data File : BN033384.D
Acq On : 14 Aug 2024 15:57
Operator : MA/JU
Sample : P3502-21
Misc :
ALS Vial : 12 Sample Multiplier: 1

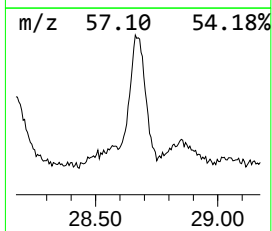
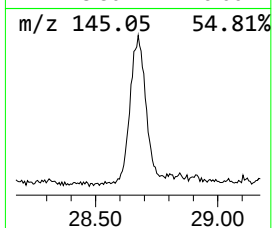
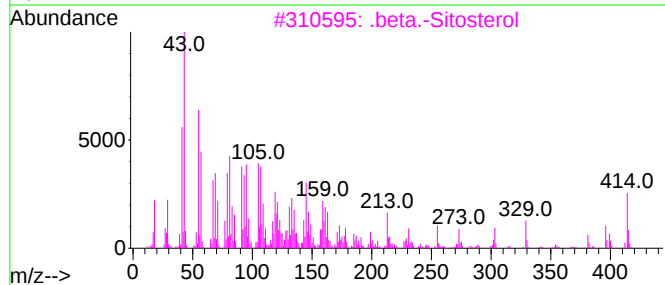
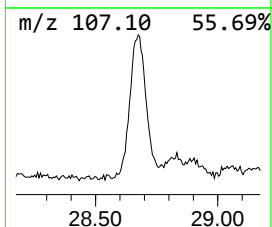
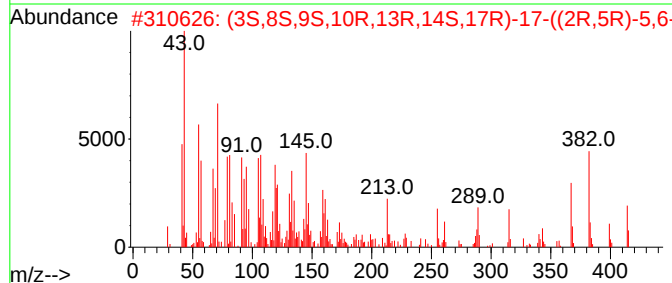
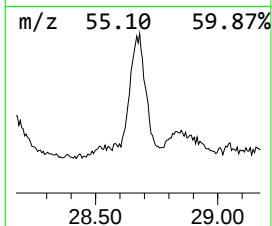
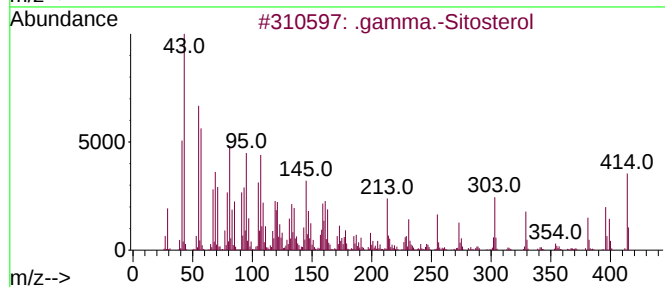
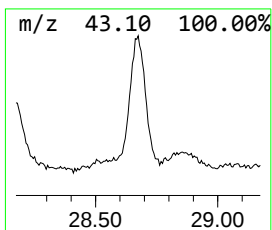
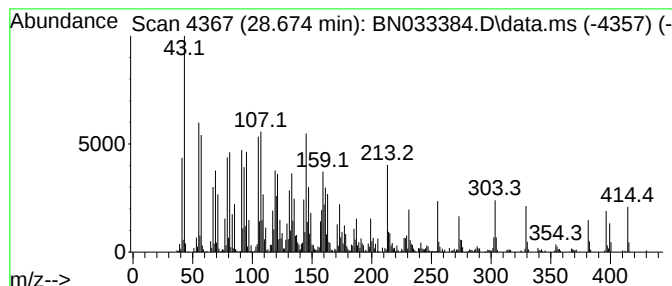
Instrument :
BNA_N
ClientSampleId :
DCXV5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 24 .gamma.-Sitosterol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.674	10.36 ng/ul	2515570	Perylene-d12	24.027	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
2	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	89
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	89
4	.beta.-Sitosterol	414	C29H50O	000083-46-5	70
5	Campesterol	400	C28H48O	000474-62-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081424\
 Data File : BN033384.D
 Acq On : 14 Aug 2024 15:57
 Operator : MA/JU
 Sample : P3502-21
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 DCXV5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
 Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.405	3.4	ng/ul	314209	1	7.569	1868230	20.0
.alpha.-Pinene	6.287	17.0	ng/ul	1591150	1	7.569	1868230	20.0
1-Phenoxypropan...	11.081	3.4	ng/ul	507809	2	10.334	2988850	20.0
(1R,2S,6S,7S,8S...	13.104	2.0	ng/ul	644580	3	14.210	6294050	20.0
1-Naphthalenol,...	15.710	4.6	ng/ul	1150980	4	16.957	5021310	20.0
n-Hexadecanoic ...	17.898	10.7	ng/ul	2677860	4	16.957	5021310	20.0
n-Propyl 11-oct...	19.063	2.3	ng/ul	578055	4	16.957	5021310	20.0
Octadecanoic acid	19.186	6.4	ng/ul	1701540	5	21.198	5286330	20.0
2-Propenoic aci...	19.786	4.8	ng/ul	1275160	5	21.198	5286330	20.0
Myrtenyl isoval...	19.933	4.1	ng/ul	1089290	5	21.198	5286330	20.0
2-Propenal, 3-(...	20.586	3.5	ng/ul	930089	5	21.198	5286330	20.0
Cinnamyl cinnamate	20.745	79.1	ng/ul	20917700	5	21.198	5286330	20.0
Dehydroabietic ...	20.880	9.0	ng/ul	2387150	5	21.198	5286330	20.0
(DEL) Alkane: S...	20.927	11.4	ng/ul	3016850	5	21.198	5286330	20.0
Docosanoic acid	21.269	3.1	ng/ul	823749	5	21.198	5286330	20.0
Pentadecafluoro...	21.439	3.0	ng/ul	791527	5	21.198	5286330	20.0
(DEL) Alkane: S...	22.004	26.8	ng/ul	7069580	5	21.198	5286330	20.0
Tetracosanoic acid	22.416	3.4	ng/ul	890504	5	21.198	5286330	20.0
(DEL) Alkane: C...	22.633	3.3	ng/ul	796294	6	24.027	4854380	20.0
(DEL) Alkane: S...	23.327	11.2	ng/ul	2714900	6	24.027	4854380	20.0
1-Heneicosanol	23.363	10.6	ng/ul	2583440	6	24.027	4854380	20.0
(DEL) Alkane: S...	25.151	20.2	ng/ul	4907510	6	24.027	4854380	20.0
1-Heptacosanol	25.245	7.7	ng/ul	1871140	6	24.027	4854380	20.0
.gamma.-Sitosterol	28.674	10.4	ng/ul	2515570	6	24.027	4854380	20.0