

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
 Data File : BP018380.D
 Acq On : 25 Nov 2023 22:06
 Operator : MA/JU
 Sample : 05261-07
 Misc :
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCKQ6

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_P\Methods\SFAM-EPA-BP112223.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP018380.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.270	27	31	39	rVB	69922	86030	0.97%	0.102%
2	3.558	76	80	86	rVB	20810	28146	0.32%	0.033%
3	3.693	99	103	111	rBV2	104897	172127	1.93%	0.205%
4	3.805	118	122	128	rVV	78252	92792	1.04%	0.110%
5	3.881	132	135	139	rVV3	17852	24360	0.27%	0.029%
6	3.934	139	144	151	rVB	60992	94564	1.06%	0.112%
7	4.028	157	160	164	rVB2	25594	35252	0.40%	0.042%
8	4.405	220	224	230	rVB4	21476	29855	0.33%	0.035%
9	4.952	312	317	324	rBV	95526	149829	1.68%	0.178%
10	5.846	465	469	475	rBV2	18853	27026	0.30%	0.032%
11	6.546	581	588	595	rBV	217733	335361	3.76%	0.399%
12	6.846	632	639	644	rBV5	29887	60829	0.68%	0.072%
13	7.028	661	670	684	rVB	991064	1790864	20.09%	2.129%
14	7.199	692	699	707	rVB	921744	1400007	15.71%	1.664%
15	7.393	725	732	740	rBV	1075661	1649283	18.50%	1.960%
16	7.463	740	744	748	rBV	73690	109426	1.23%	0.130%
17	7.863	805	812	820	rBV	1350597	2115072	23.73%	2.514%
18	8.569	924	932	942	rBV	756414	1221333	13.70%	1.452%
19	8.687	945	952	960	rVV	431523	689212	7.73%	0.819%
20	8.805	965	972	980	rVB	46466	89755	1.01%	0.107%
21	9.022	1002	1009	1017	rBV	930601	1497573	16.80%	1.780%
22	9.269	1045	1051	1059	rVB4	13747	26901	0.30%	0.032%
23	9.463	1079	1084	1088	rVB3	21025	33639	0.38%	0.040%
24	9.746	1124	1132	1139	rBV	655153	1060675	11.90%	1.261%
25	9.899	1148	1158	1168	rBV	133251	298515	3.35%	0.355%
26	10.104	1185	1193	1199	rBV	74001	124852	1.40%	0.148%
27	10.281	1216	1223	1231	rBV	1136105	1819510	20.41%	2.163%
28	10.663	1281	1288	1295	rBV	1649822	2686747	30.14%	3.194%
29	10.804	1306	1312	1325	rVB	118267	234396	2.63%	0.279%
30	11.146	1366	1370	1374	rBV	25938	40223	0.45%	0.048%
31	11.199	1374	1379	1386	rVB4	54648	90418	1.01%	0.107%
32	11.446	1415	1421	1426	rBV	38936	68946	0.77%	0.082%
33	12.028	1514	1520	1524	rBV	19241	30061	0.34%	0.036%
34	12.251	1547	1558	1562	rBV3	26932	49436	0.55%	0.059%
35	12.869	1659	1663	1673	rVV2	68557	112202	1.26%	0.133%
36	13.245	1722	1727	1730	rBV5	22938	41449	0.46%	0.049%

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112223.MA.M
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37	13.404	1746	1754	1760	rVV	508490	850680	9.54%	1.011%
38	13.581	1779	1784	1791	rBV	28604	44032	0.49%	0.052%
39	13.828	1821	1826	1831	rVB3	112411	158755	1.78%	0.189%
40	13.910	1834	1840	1851	rVB	1805154	2423288	27.19%	2.880%
41	14.192	1876	1888	1896	rBV	1983983	3050455	34.22%	3.626%
42	14.263	1897	1900	1905	rVV6	18025	31856	0.36%	0.038%
43	14.345	1907	1914	1920	rVV5	51043	84239	0.95%	0.100%
44	14.498	1926	1940	1946	rVV	1970388	3128087	35.09%	3.718%
45	14.575	1948	1953	1961	rVB4	59594	127761	1.43%	0.152%
46	14.687	1966	1972	1979	rBV	523040	800556	8.98%	0.952%
47	14.757	1980	1984	1991	rVV3	52218	120990	1.36%	0.144%
48	14.840	1991	1998	2004	rVV2	86780	202088	2.27%	0.240%
49	14.916	2004	2011	2017	rVB8	24324	54506	0.61%	0.065%
50	15.487	2102	2108	2115	rBV	2528445	3660779	41.07%	4.351%
51	15.598	2121	2127	2138	rVV	383891	534619	6.00%	0.635%
52	15.692	2139	2143	2146	rVV6	13733	24928	0.28%	0.030%
53	15.734	2146	2150	2156	rVB6	19890	33076	0.37%	0.039%
54	15.834	2162	2167	2171	rBV4	51938	81497	0.91%	0.097%
55	15.916	2177	2181	2185	rVV6	30239	48644	0.55%	0.058%
56	15.981	2186	2192	2198	rVB	179136	270810	3.04%	0.322%
57	16.069	2203	2207	2214	rVB8	33570	61195	0.69%	0.073%
58	16.222	2227	2233	2236	rBV2	25467	40050	0.45%	0.048%
59	16.345	2250	2254	2257	rBV5	20436	28053	0.31%	0.033%
60	16.381	2257	2260	2268	rVB6	33452	58083	0.65%	0.069%
61	16.786	2326	2329	2337	rBV4	17891	37491	0.42%	0.045%
62	17.245	2401	2407	2412	rBV	2183121	3106077	34.85%	3.692%
63	17.286	2412	2414	2418	rVV	219608	260889	2.93%	0.310%
64	17.345	2418	2424	2434	rVB	2095127	3025473	33.94%	3.596%
65	17.445	2434	2441	2446	rVB	28048	53345	0.60%	0.063%
66	17.645	2473	2475	2482	rVB	18748	29737	0.33%	0.035%
67	17.751	2490	2493	2499	rBV5	24506	33574	0.38%	0.040%
68	17.933	2520	2524	2528	rVB	45549	55332	0.62%	0.066%
69	18.010	2532	2537	2545	rVB4	46431	106111	1.19%	0.126%
70	18.086	2546	2550	2553	rBV	66763	94268	1.06%	0.112%
71	18.145	2553	2560	2569	rVV2	654938	934283	10.48%	1.111%
72	18.298	2583	2586	2590	rVB3	34435	44348	0.50%	0.053%
73	18.457	2606	2613	2621	rVB4	61384	129720	1.46%	0.154%
74	18.598	2634	2637	2641	rBV2	81880	112046	1.26%	0.133%
75	18.698	2650	2654	2661	rVB	125397	162786	1.83%	0.193%
76	18.916	2687	2691	2695	rBV	95642	123820	1.39%	0.147%

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 Title : SVOA CALIBRATION

77	18.957	2695	2698	2702	rVB	44355	45962	0.52%	0.055%
78	19.004	2702	2706	2709	rBV2	78202	102550	1.15%	0.122%
79	19.069	2709	2717	2720	rBV4	130066	218528	2.45%	0.260%
80	19.139	2725	2729	2730	rBV3	60909	70904	0.80%	0.084%
81	19.257	2745	2749	2754	rVB	399198	559957	6.28%	0.666%
82	19.380	2767	2770	2781	rBV	238380	327325	3.67%	0.389%
83	19.586	2799	2805	2815	rBV	3465626	5011769	56.22%	5.957%
84	19.886	2853	2856	2860	rBV2	89572	105947	1.19%	0.126%
85	19.980	2866	2872	2877	rVB2	169277	269959	3.03%	0.321%
86	20.104	2889	2893	2894	rBV2	84590	101190	1.14%	0.120%
87	20.127	2894	2897	2905	rVB5	192805	329920	3.70%	0.392%
88	20.527	2962	2965	2968	rVB3	53969	61967	0.70%	0.074%
89	20.710	2994	2996	3000	rVB3	68619	69072	0.77%	0.082%
90	20.763	3002	3005	3009	rBV	258778	277192	3.11%	0.329%
91	20.922	3027	3032	3041	rVB	7868669	8913813	100.00%	10.595%
92	21.092	3056	3061	3070	rBV2	1204777	1768737	19.84%	2.102%
93	21.357	3100	3106	3110	rBV	3122169	4231400	47.47%	5.030%
94	21.398	3110	3113	3123	rVB2	358080	523621	5.87%	0.622%
95	21.551	3137	3139	3143	rBV2	123081	149218	1.67%	0.177%
96	22.051	3218	3224	3236	rBV	1521767	2696394	30.25%	3.205%
97	23.186	3410	3417	3422	rBV	1639625	3826406	42.93%	4.548%
98	23.633	3487	3493	3500	rBV2	2158026	4309597	48.35%	5.123%
99	23.798	3514	3521	3529	rBV	2052598	4297619	48.21%	5.108%
100	24.739	3672	3681	3690	rBV	920221	3214857	36.07%	3.821%

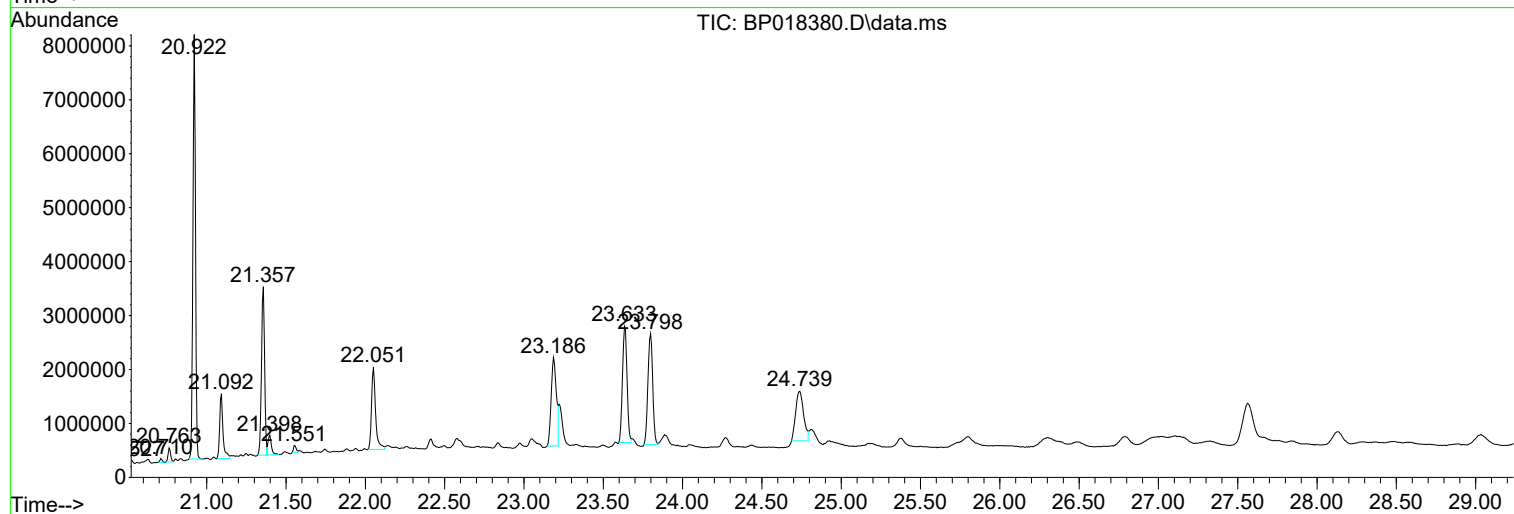
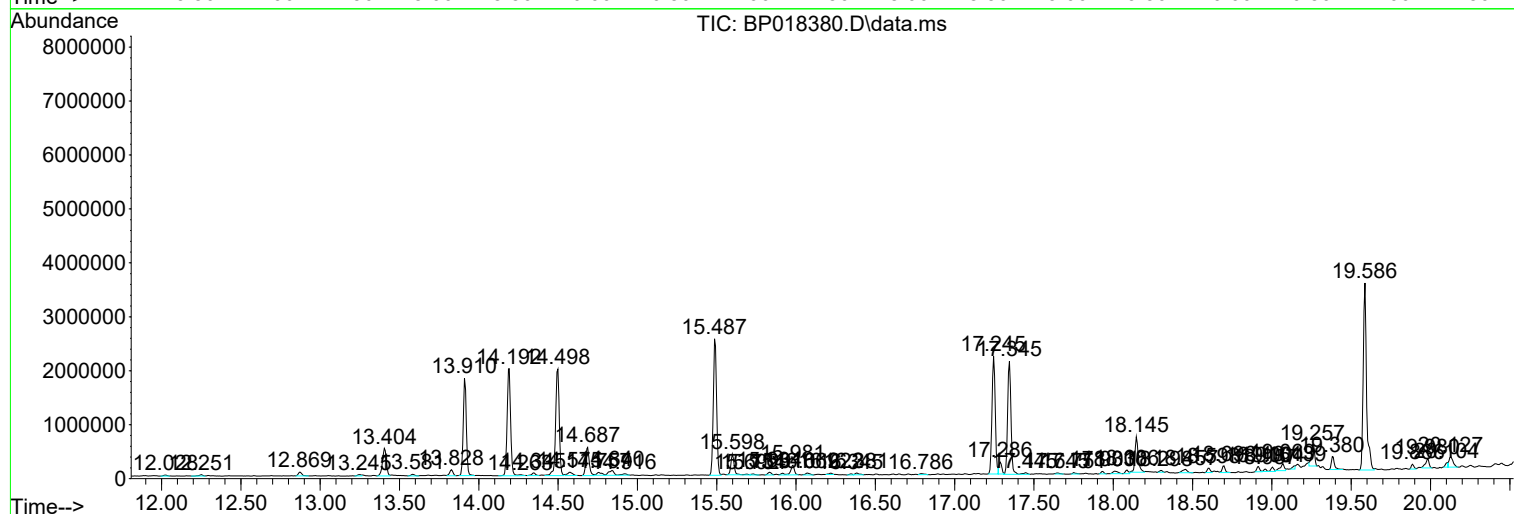
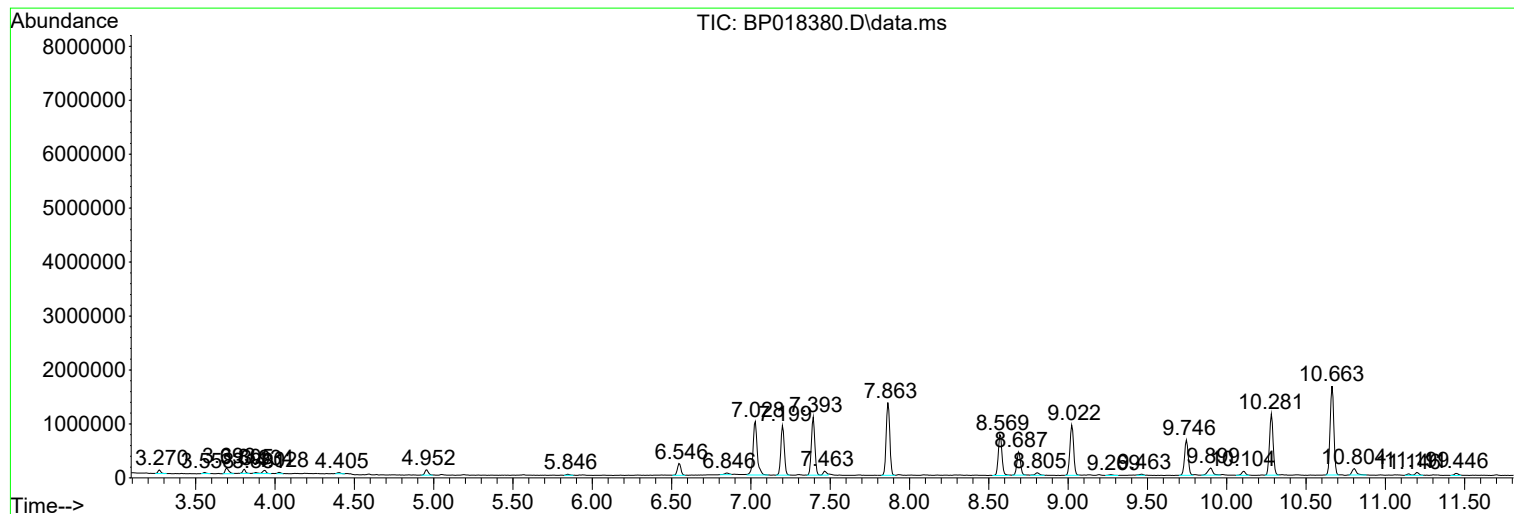
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112223.MA.M
Quant Title : SVOA CALIBRATION

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



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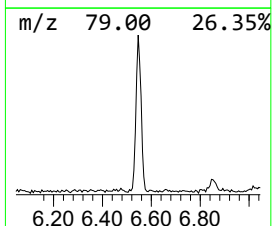
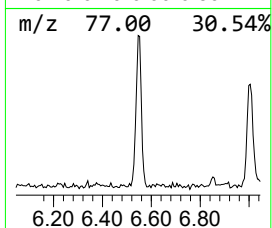
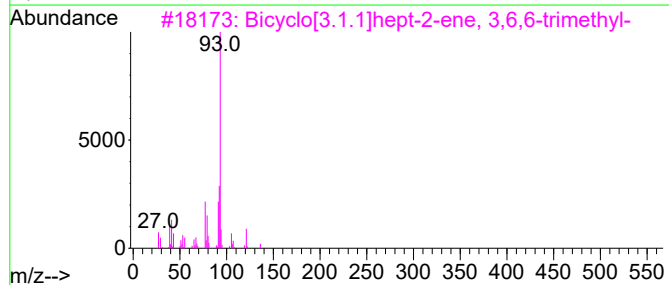
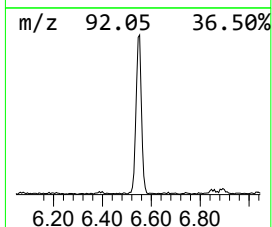
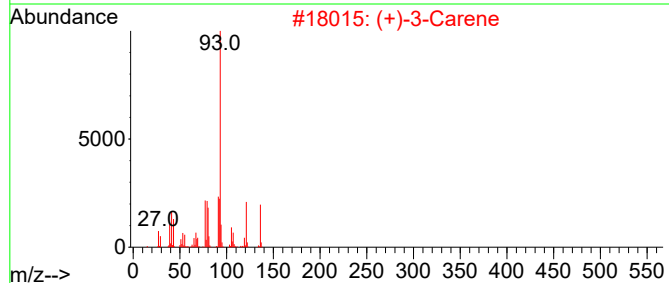
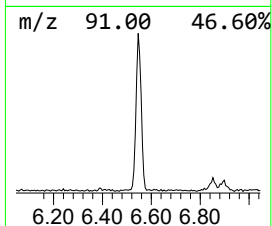
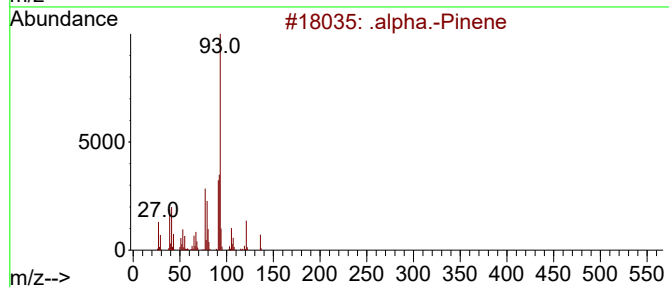
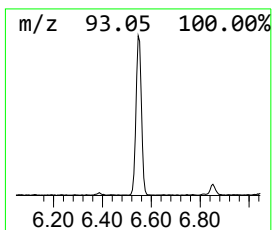
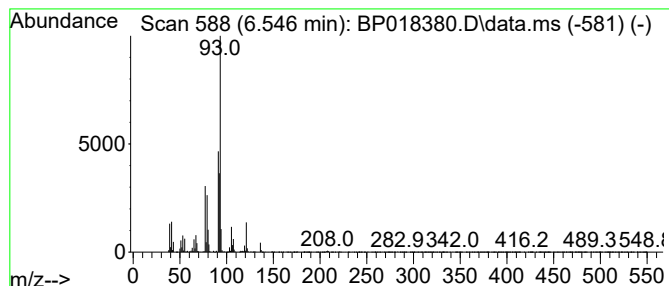
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112223.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 .alpha.-Pinene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.546	3.17 ng/ul	335361	1,4-Dichlorobenzene-d4	7.863

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



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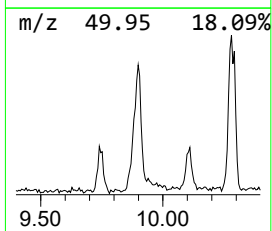
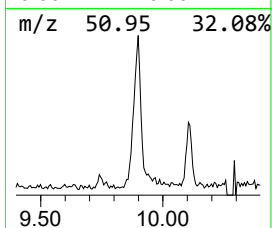
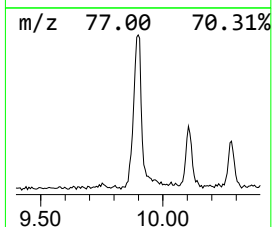
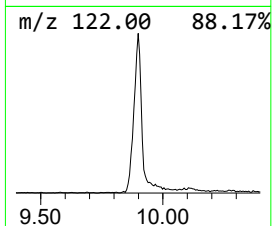
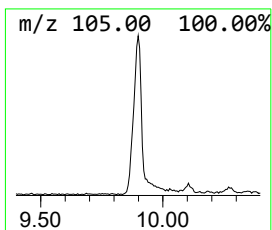
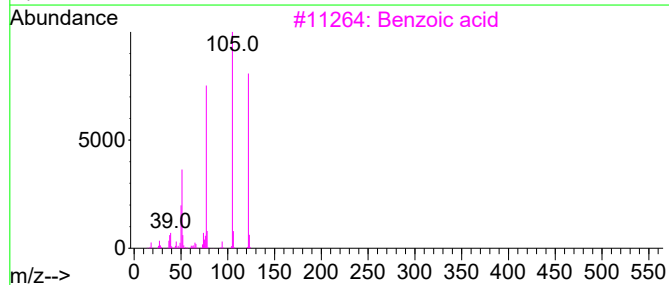
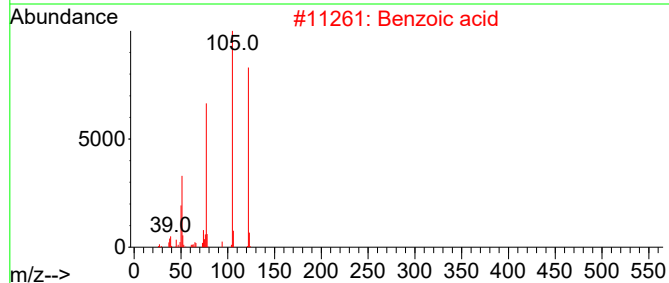
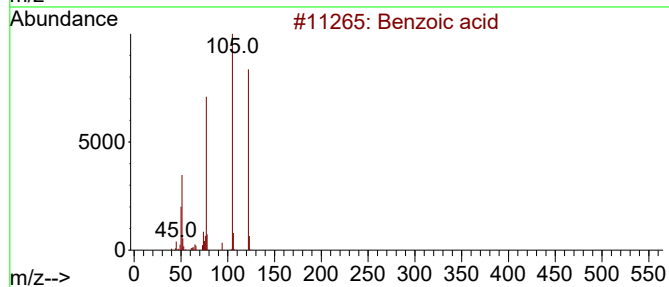
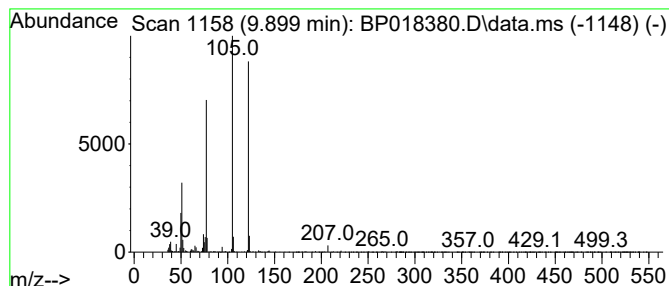
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP112223.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.899	2.22 ng/ul	298515	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid			122	C7H6O2	000065-85-0	96
2	Benzoic acid			122	C7H6O2	000065-85-0	94
3	Benzoic acid			122	C7H6O2	000065-85-0	94
4	Benzoic acid			122	C7H6O2	000065-85-0	94
5	Benzoic acid, silver(1+) salt			228	C7H5AgO2	000532-31-0	90



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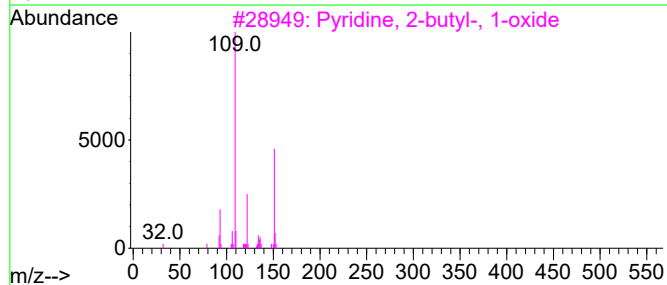
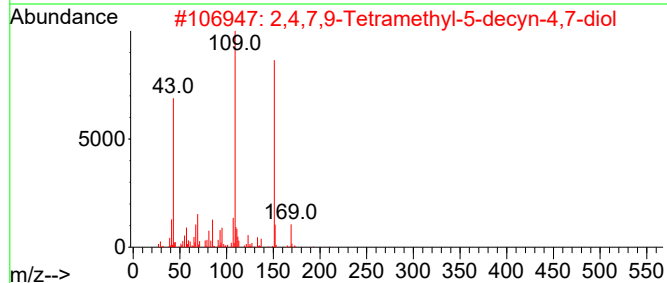
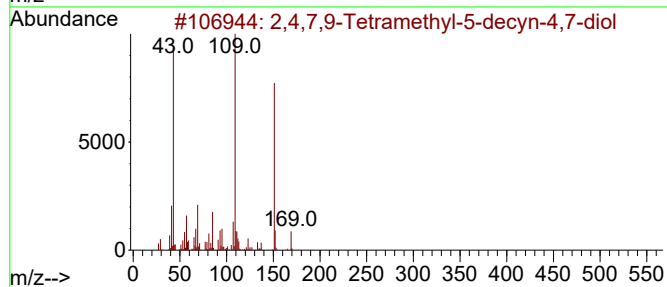
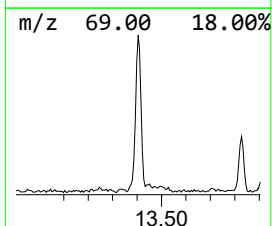
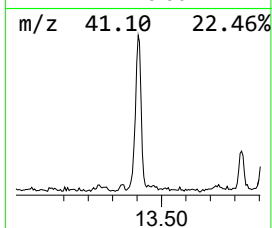
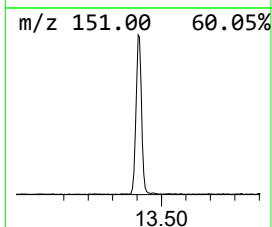
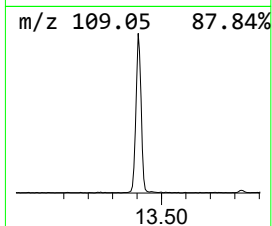
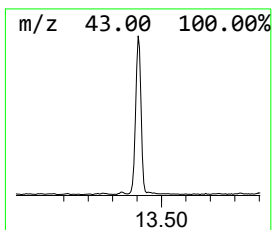
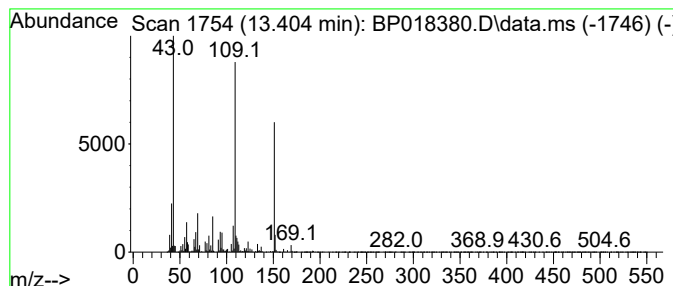
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.404	5.44 ng/ul	850680	Acenaphthene-d10	14.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91		
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90		
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59		
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	59		
5	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
Data File : BP018380.D
Acq On : 25 Nov 2023 22:06
Operator : MA/JU
Sample : 05261-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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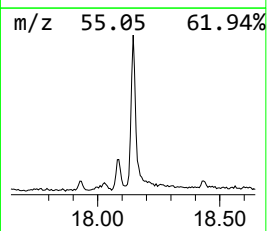
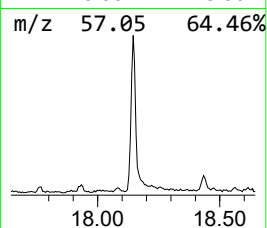
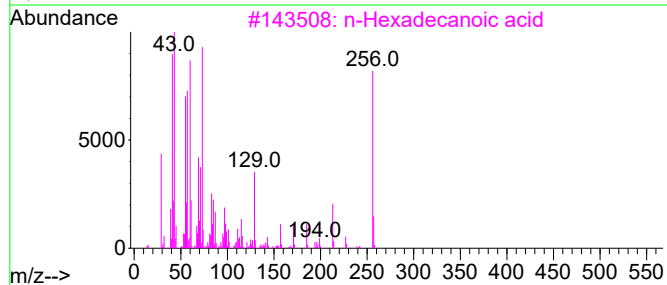
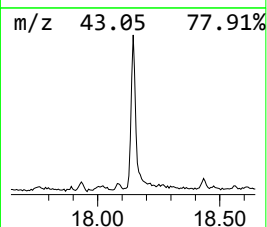
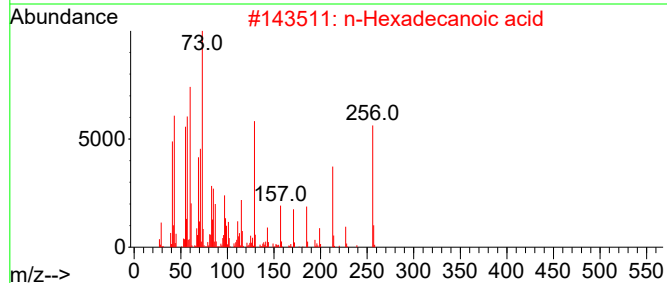
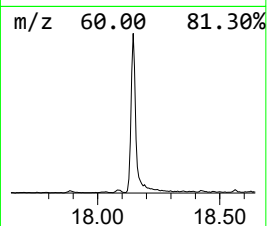
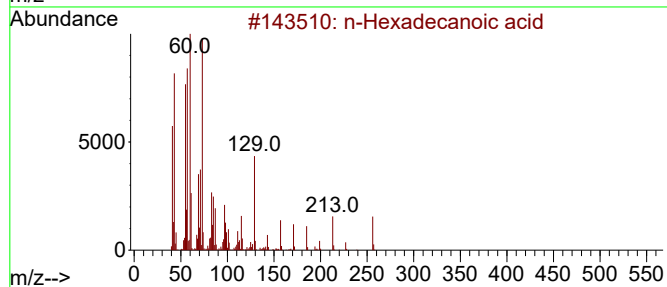
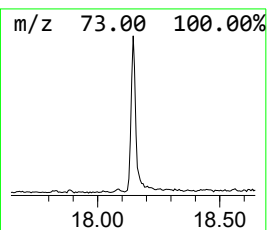
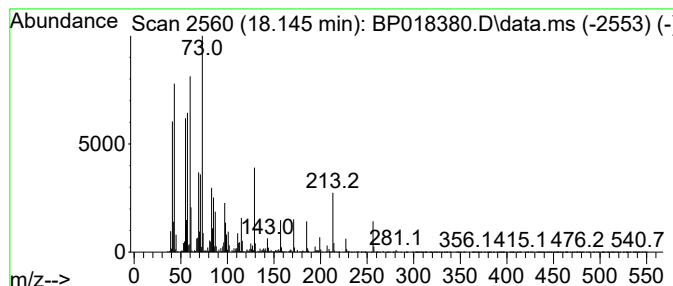
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	6.02 ng/ul	934283	Phenanthrene-d10	17.245

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			Tridecanoic acid	214	C13H26O2	000638-53-9	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
Data File : BP018380.D
Acq On : 25 Nov 2023 22:06
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Sample : 05261-07
Misc :
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ClientSampleId :
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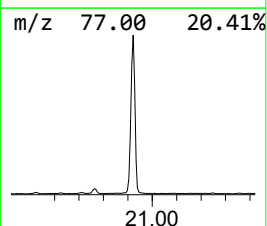
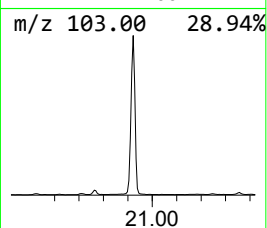
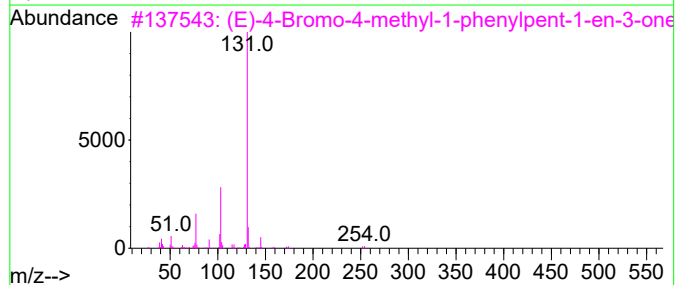
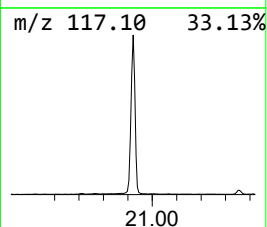
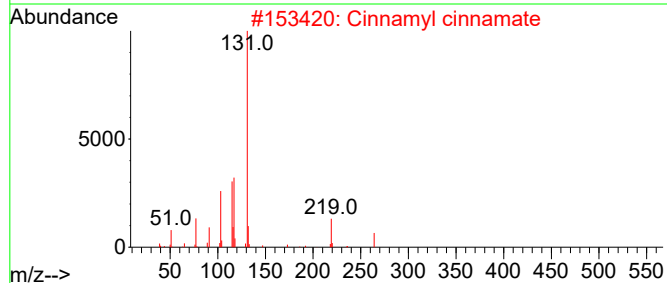
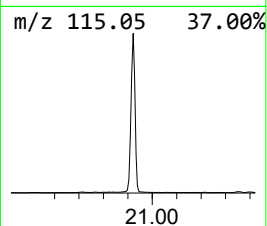
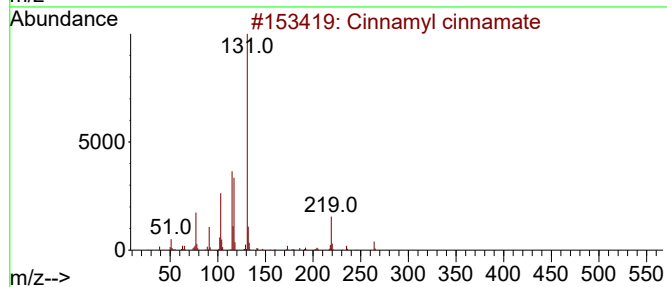
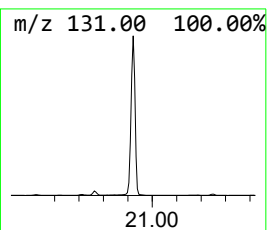
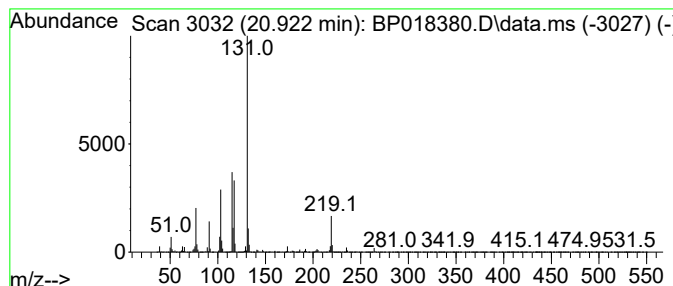
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.922	42.13 ng/ul	8913810	Chrysene-d12	21.357

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			(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	53
4			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52
5			N-(4-Fluorophenyl)-3-phenyl-2-pr...	337	C17H11F4NO2	1000492-37-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
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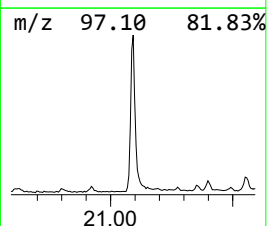
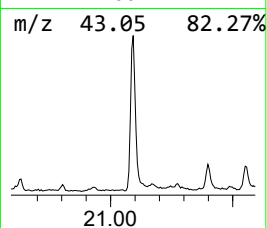
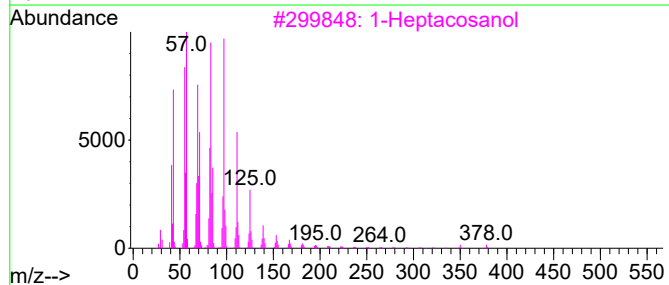
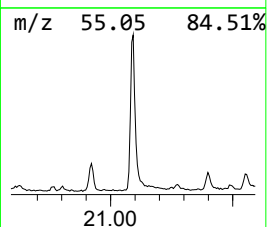
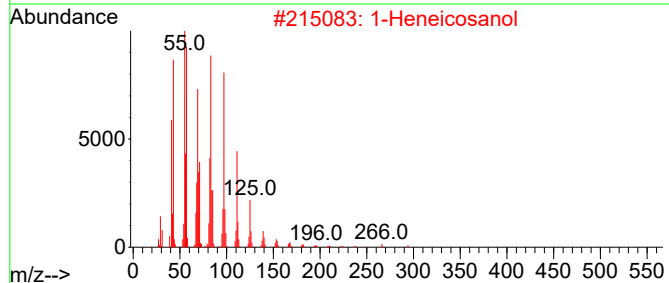
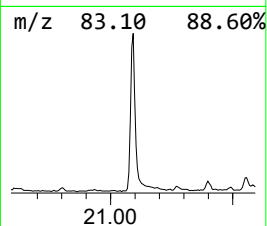
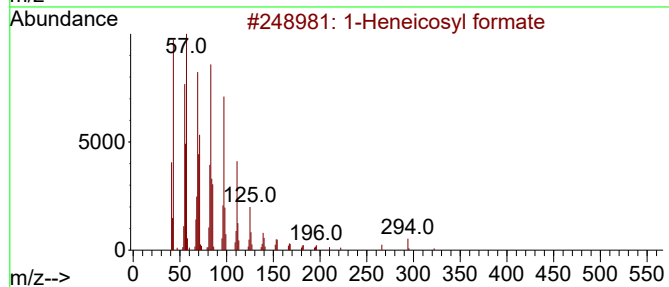
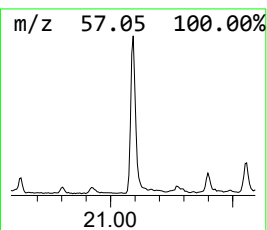
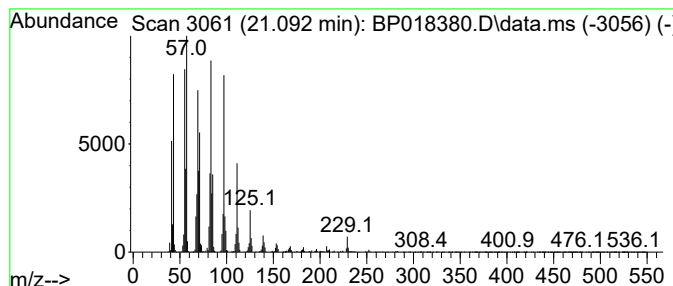
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	8.36 ng/ul	1768740	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	97
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			1-Heptacosanol	396	C27H56O	002004-39-9	95
4			1-Hexacosene	364	C26H52	018835-33-1	95
5			Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
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Sample : 05261-07
Misc :
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Instrument :
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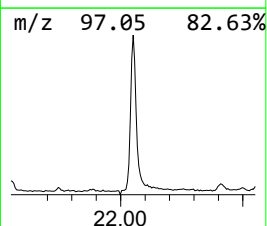
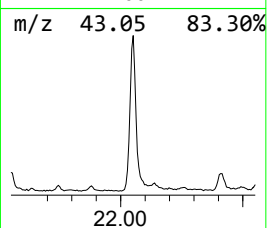
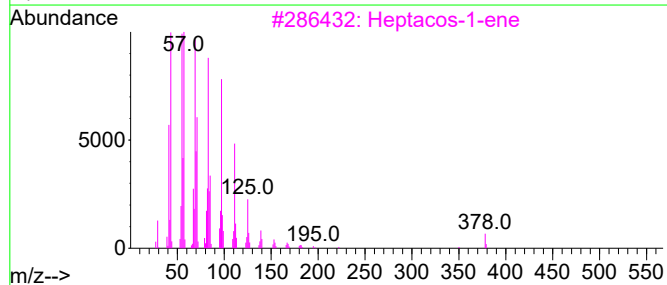
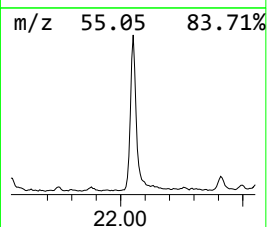
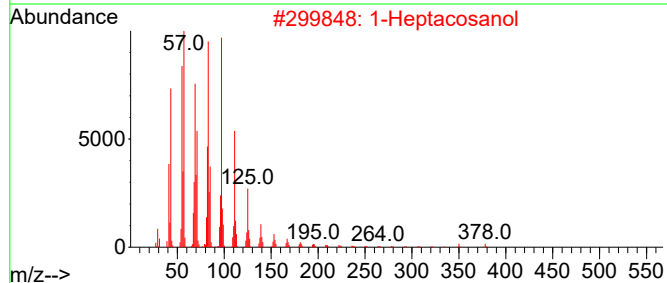
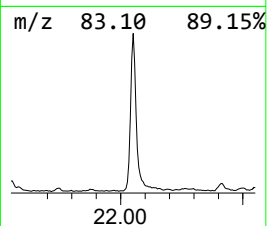
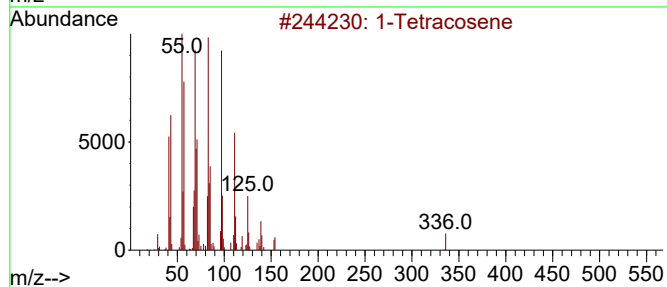
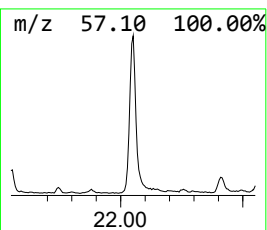
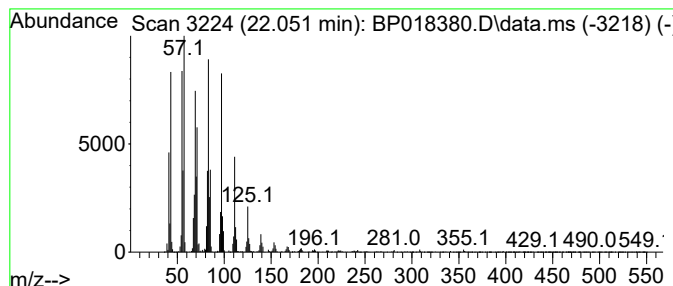
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.051	12.74 ng/ul	2696390	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene			336	C24H48	010192-32-2	99
2	1-Heptacosanol			396	C27H56O	002004-39-9	95
3	Heptacos-1-ene			378	C27H54	015306-27-1	94
4	1-Hexacosene			364	C26H52	018835-33-1	93
5	Octacosanol			410	C28H58O	000557-61-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
Data File : BP018380.D
Acq On : 25 Nov 2023 22:06
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Sample : 05261-07
Misc :
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Instrument :
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ClientSampleId :
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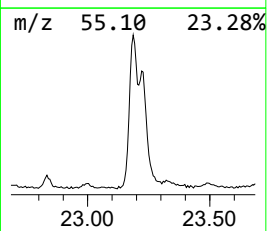
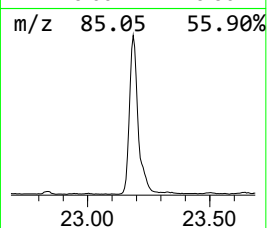
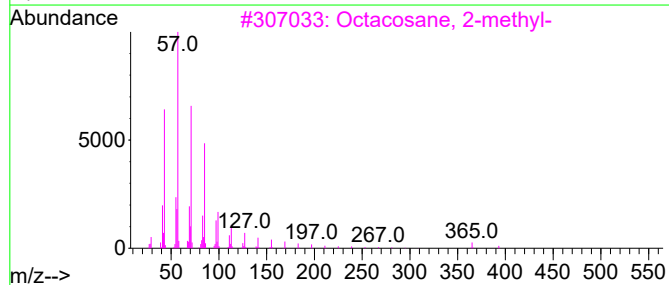
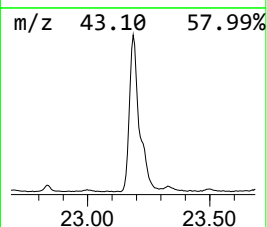
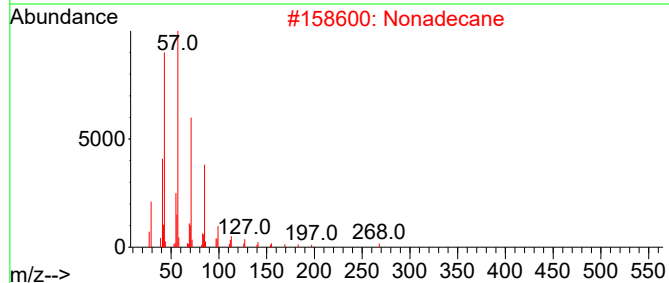
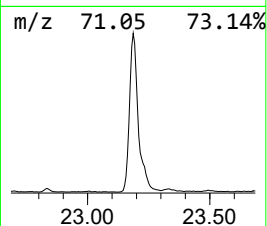
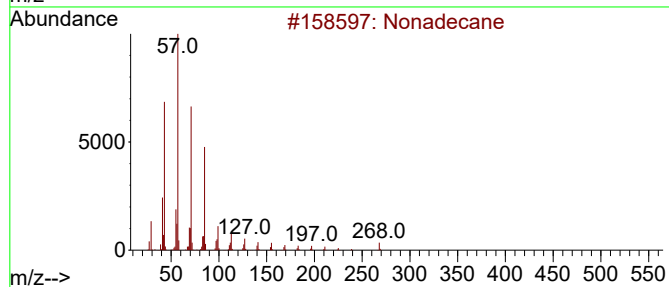
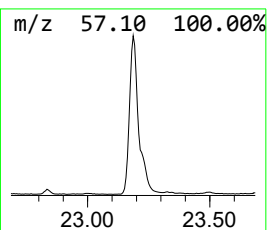
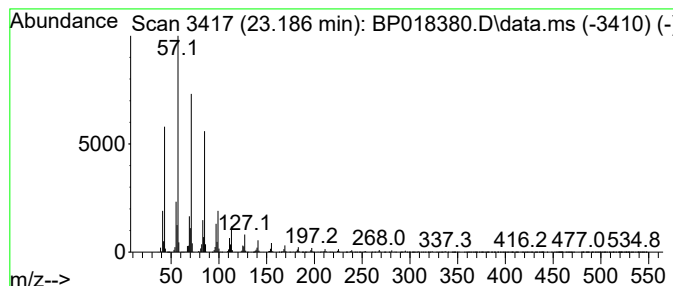
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.186	17.81 ng/ul	3826410	Perylene-d12	23.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	95
2			Nonadecane	268	C19H40	000629-92-5	95
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
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Sample : 05261-07
Misc :
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ClientSampleId :
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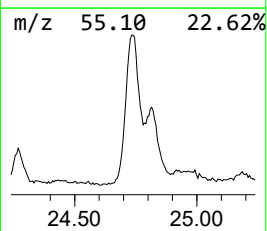
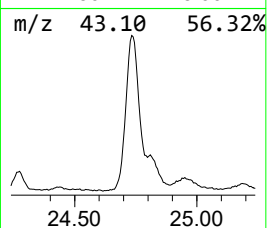
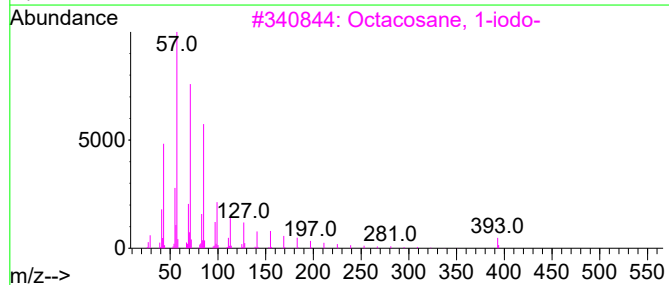
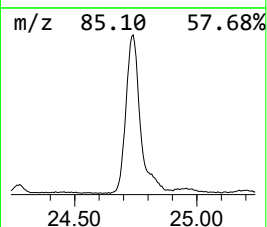
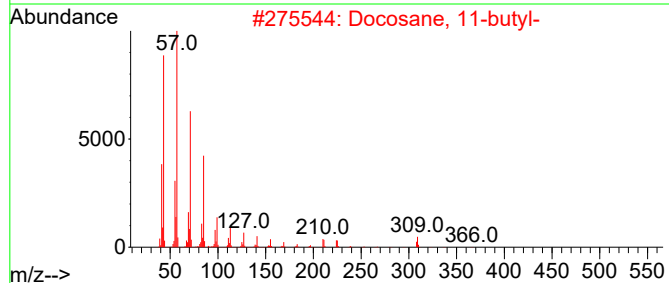
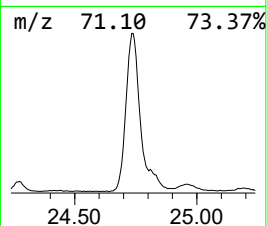
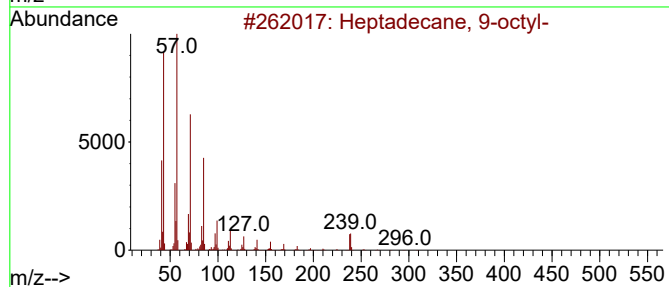
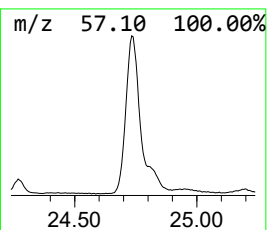
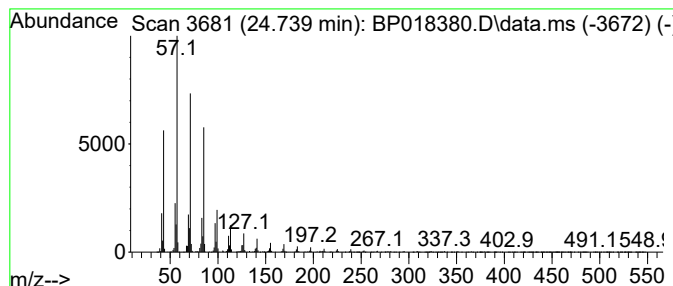
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.739	14.96 ng/ul	3214860	Perylene-d12	23.798

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	93
3		Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	91
4		Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91
5		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112423\
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Sample : 05261-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzoic acid	9.899	2.2	ng/ul	298515	2	10.663	2686750	20.0
2,4,7,9-Tetrame...	13.404	5.4	ng/ul	850680	3	14.498	3128090	20.0
n-Hexadecanoic ...	18.145	6.0	ng/ul	934283	4	17.245	3106080	20.0
Cinnamyl cinnamate	20.922	42.1	ng/ul	8913810	5	21.357	4231400	20.0
1-Heneicosyl fo...	21.092	8.4	ng/ul	1768740	5	21.357	4231400	20.0
(DEL) Alkane: S...	22.051	12.7	ng/ul	2696390	5	21.357	4231400	20.0
(DEL) Alkane: S...	23.186	17.8	ng/ul	3826410	6	23.798	4297620	20.0
(DEL) Alkane: S...	24.739	15.0	ng/ul	3214860	6	23.798	4297620	20.0