

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
 Data File : BP013153.D
 Acq On : 20 Dec 2022 07:24
 Operator : CG/JU
 Sample : N6003-02
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DBXX1

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-BP120722.M
 Title : SVOA CALIBRATION

Signal : TIC: BP013153.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	22	25	36	rVB	168579	228255	1.85%	0.143%
2	3.623	71	74	82	rVB	63560	82694	0.67%	0.052%
3	3.770	95	99	113	rBV	912471	1399279	11.32%	0.876%
4	3.870	113	116	123	rVB2	55977	76782	0.62%	0.048%
5	3.999	133	138	142	rVB	71515	102958	0.83%	0.064%
6	4.093	150	154	161	rVB	44649	65705	0.53%	0.041%
7	4.475	216	219	225	rVB4	18322	24737	0.20%	0.015%
8	4.664	247	251	256	rVB3	26857	38815	0.31%	0.024%
9	5.040	309	315	323	rVV	464303	670910	5.43%	0.420%
10	5.128	327	330	336	rVB6	16467	22826	0.18%	0.014%
11	5.281	353	356	363	rVB5	14788	22786	0.18%	0.014%
12	6.928	632	636	642	rBV4	21576	33930	0.27%	0.021%
13	7.111	659	667	682	rBV	2690175	4230620	34.22%	2.647%
14	7.281	689	696	706	rVB	2295690	3479770	28.14%	2.177%
15	7.481	723	730	740	rBV	2770485	4276696	34.59%	2.676%
16	7.564	740	744	750	rVB8	17919	30730	0.25%	0.019%
17	7.952	803	810	818	rBV	2132002	3398666	27.49%	2.127%
18	8.016	818	821	826	rVB2	14623	22587	0.18%	0.014%
19	8.175	842	848	850	rBV7	21058	32416	0.26%	0.020%
20	8.663	921	931	940	rBV	3048188	4828746	39.05%	3.021%
21	8.781	946	951	959	rVB	112381	188158	1.52%	0.118%
22	9.122	1001	1009	1019	rBV	2553194	4173098	33.75%	2.611%
23	9.281	1031	1036	1044	rVB7	23510	42992	0.35%	0.027%
24	9.528	1071	1078	1083	rVB2	64791	111671	0.90%	0.070%
25	9.693	1102	1106	1114	rVB4	16095	29141	0.24%	0.018%
26	9.846	1123	1132	1149	rBV	2220751	3572576	28.89%	2.235%
27	9.987	1152	1156	1164	rVV6	16461	36133	0.29%	0.023%
28	10.063	1164	1169	1175	rVB8	13993	26871	0.22%	0.017%
29	10.387	1216	1224	1240	rBV	3125286	5246213	42.43%	3.283%
30	10.546	1246	1251	1259	rVB10	16463	37478	0.30%	0.023%
31	10.769	1281	1289	1296	rBV	2878501	4714786	38.13%	2.950%
32	10.905	1301	1312	1334	rVV	1578098	2975986	24.07%	1.862%
33	11.299	1373	1379	1386	rVB10	19145	39462	0.32%	0.025%
34	11.552	1416	1422	1431	rVB8	22682	47310	0.38%	0.030%
35	12.181	1522	1529	1536	rVV7	16170	27983	0.23%	0.018%
36	12.287	1543	1547	1552	rVV	37970	65425	0.53%	0.041%

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
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37	12.351	1554	1558	1567	rVB2	59163	97879	0.79%	0.061%
38	12.963	1657	1662	1667	rBV8	15255	30753	0.25%	0.019%
39	13.410	1729	1738	1744	rVB3	39091	61325	0.50%	0.038%
40	13.481	1744	1750	1754	rBV8	14562	25131	0.20%	0.016%
41	13.575	1761	1766	1772	rVB8	12373	26532	0.21%	0.017%
42	13.775	1794	1800	1807	rBV8	11202	25832	0.21%	0.016%
43	13.916	1818	1824	1829	rBV	151510	213301	1.73%	0.133%
44	14.004	1832	1839	1847	rBV	4762899	6613650	53.49%	4.138%
45	14.069	1847	1850	1853	rVV4	19170	27296	0.22%	0.017%
46	14.116	1854	1858	1862	rVB7	15247	24440	0.20%	0.015%
47	14.234	1873	1878	1881	rBV7	14241	29754	0.24%	0.019%
48	14.293	1881	1888	1899	rVV	5625166	8333106	67.40%	5.214%
49	14.481	1916	1920	1925	rVB	32658	44353	0.36%	0.028%
50	14.593	1933	1939	1947	rBV	3722459	5616283	45.42%	3.514%
51	14.663	1948	1951	1959	rVB10	18015	42894	0.35%	0.027%
52	14.787	1965	1972	1992	rBV	1614303	2639345	21.35%	1.651%
53	14.945	1995	1999	2004	rVV3	67889	120594	0.98%	0.075%
54	15.004	2004	2009	2016	rVV6	59601	131113	1.06%	0.082%
55	15.169	2033	2037	2042	rBV2	23510	31954	0.26%	0.020%
56	15.381	2069	2073	2076	rBV4	11635	19411	0.16%	0.012%
57	15.434	2080	2082	2087	rVB2	21632	25422	0.21%	0.016%
58	15.587	2101	2108	2115	rBV	6566157	9882879	79.93%	6.184%
59	15.645	2115	2118	2122	rVV	43519	62239	0.50%	0.039%
60	15.704	2122	2128	2140	rVV	2007993	2722727	22.02%	1.704%
61	15.828	2145	2149	2156	rVB2	39855	73451	0.59%	0.046%
62	15.957	2165	2171	2175	rVB	168414	236223	1.91%	0.148%
63	16.163	2197	2206	2211	rBV	14435	36046	0.29%	0.023%
64	16.222	2213	2216	2221	rBV5	35545	43939	0.36%	0.027%
65	16.298	2225	2229	2232	rBV5	20469	32749	0.26%	0.020%
66	16.522	2263	2267	2270	rVB3	16303	22533	0.18%	0.014%
67	16.734	2300	2303	2308	rVB7	16961	21202	0.17%	0.013%
68	17.234	2384	2388	2390	rBV5	18357	24235	0.20%	0.015%
69	17.351	2402	2408	2418	rBV	4083682	5794432	46.86%	3.626%
70	17.451	2418	2425	2435	rVV	6479181	9167362	74.14%	5.736%
71	17.534	2435	2439	2446	rVV2	112709	182891	1.48%	0.114%
72	17.628	2449	2455	2464	rVV7	36336	95832	0.78%	0.060%
73	18.010	2517	2520	2523	rVB4	27579	32623	0.26%	0.020%
74	18.110	2534	2537	2542	rVB5	25574	34728	0.28%	0.022%
75	18.222	2551	2556	2567	rBV	730256	1072532	8.67%	0.671%
76	18.469	2595	2598	2609	rVB4	78234	153901	1.24%	0.096%

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 Title : SVOA CALIBRATION

77	18.634	2622	2626	2634	rBV3	120940	157775	1.28%	0.099%
78	18.722	2639	2641	2647	rVB3	64079	85582	0.69%	0.054%
79	18.786	2648	2652	2656	rBV	244830	292349	2.36%	0.183%
80	18.828	2656	2659	2663	rVB	53549	62794	0.51%	0.039%
81	19.122	2705	2709	2714	rVB2	142509	209235	1.69%	0.131%
82	19.204	2720	2723	2728	rBV	61239	104655	0.85%	0.065%
83	19.257	2729	2732	2736	rVV3	125475	165131	1.34%	0.103%
84	19.328	2739	2744	2747	rVV	101201	205724	1.66%	0.129%
85	19.357	2747	2749	2753	rVB	97678	107324	0.87%	0.067%
86	19.451	2761	2765	2773	rBV	310471	439610	3.56%	0.275%
87	19.681	2799	2804	2817	rVB	7836559	10532809	85.19%	6.590%
88	19.833	2825	2830	2835	rBV	1930180	2304689	18.64%	1.442%
89	19.951	2847	2850	2857	rBV	121483	158490	1.28%	0.099%
90	20.180	2884	2889	2895	rBV3	190791	384403	3.11%	0.241%
91	20.410	2926	2928	2934	rVB6	77167	89926	0.73%	0.056%
92	21.127	3046	3050	3061	rBV	1299806	1913485	15.48%	1.197%
93	21.439	3098	3103	3108	rBV	4631192	6044816	48.89%	3.782%
94	23.133	3387	3391	3396	rBV	741946	1135132	9.18%	0.710%
95	23.757	3490	3497	3511	rVB2	6004015	12364389	100.00%	7.737%
96	23.921	3518	3525	3536	rVB2	3518888	7282652	58.90%	4.557%
97	24.539	3624	3630	3638	rVB	1619606	3349309	27.09%	2.096%
98	24.645	3644	3648	3663	rVB	624552	1524793	12.33%	0.954%
99	26.451	3947	3955	3971	rVB	2273656	7061307	57.11%	4.418%
100	29.027	4384	4393	4404	rBV7	1499530	5563603	45.00%	3.481%

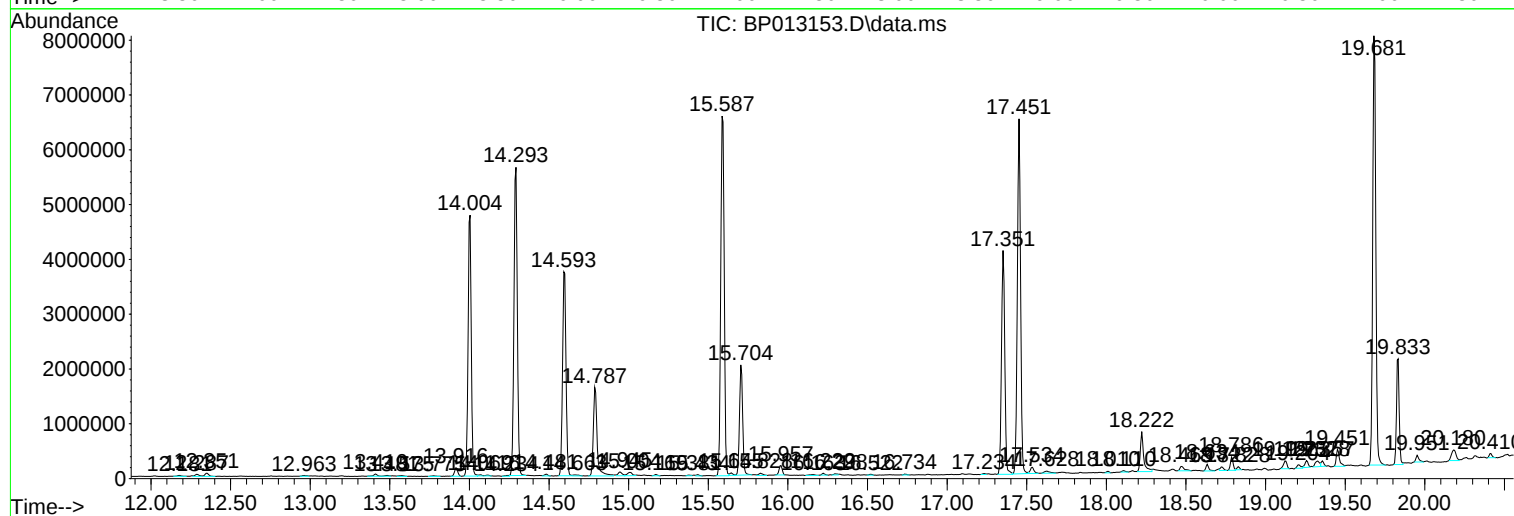
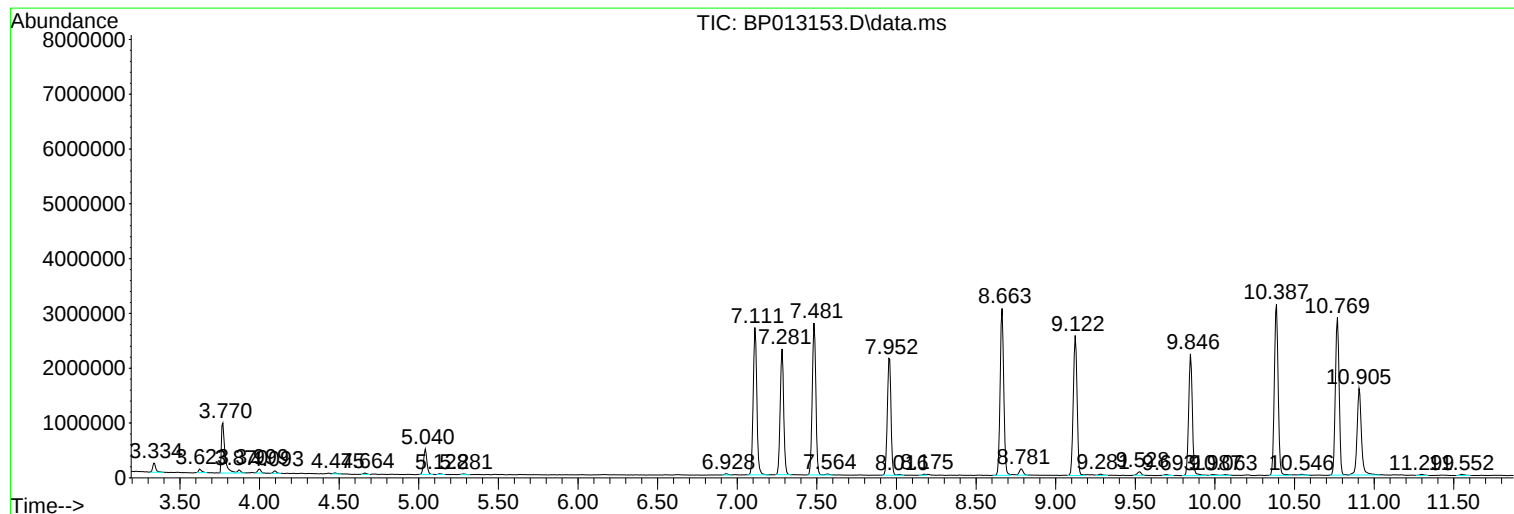
Sum of corrected areas: 159818065

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



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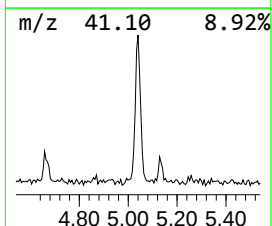
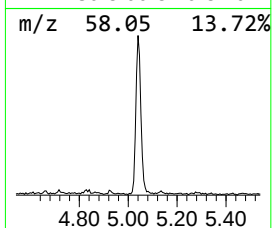
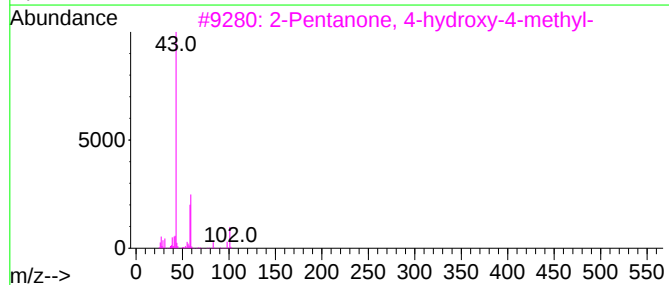
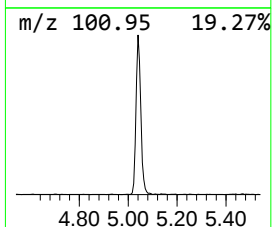
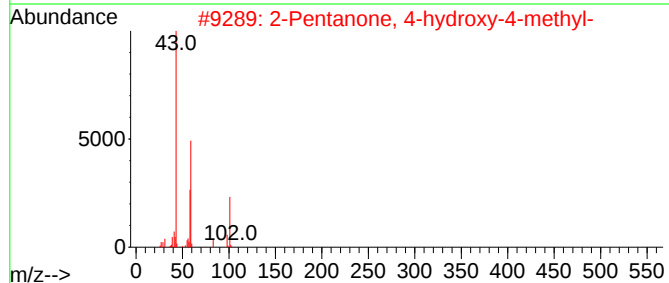
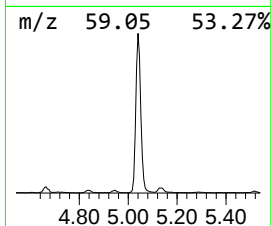
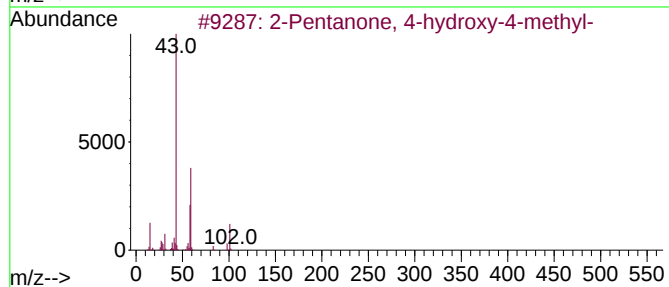
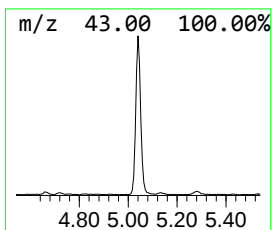
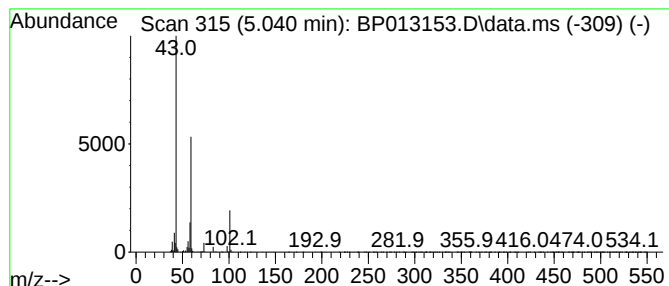
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	3.95 ng/ul	670910	1,4-Dichlorobenzene-d4	7.958

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25		



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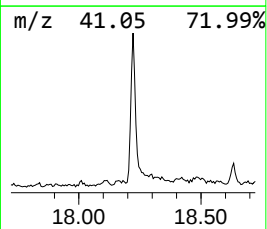
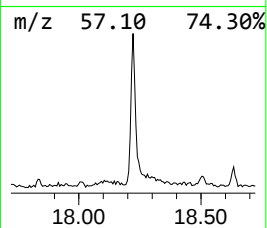
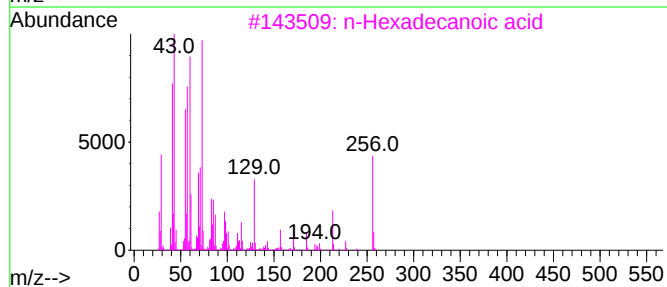
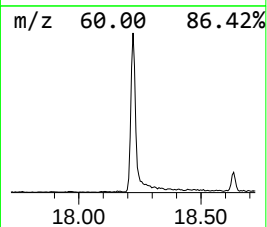
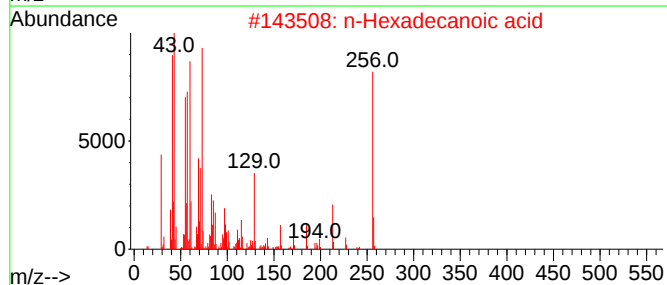
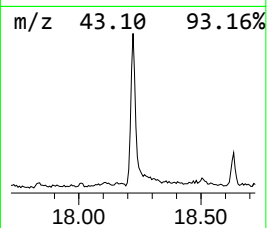
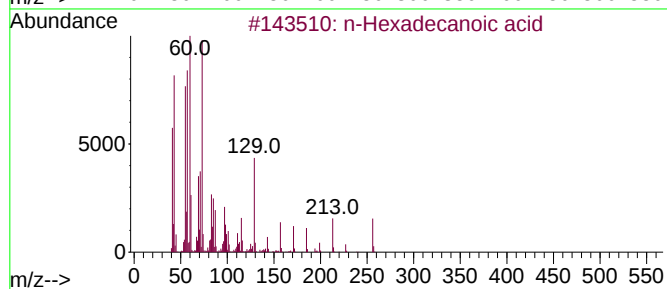
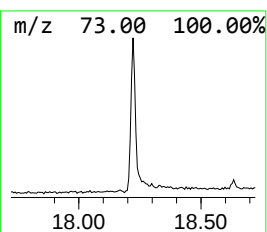
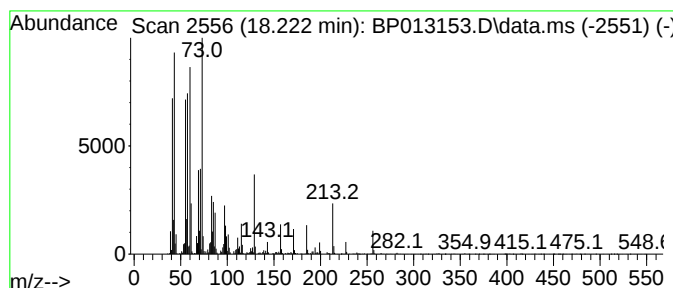
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	3.70 ng/ul	1072530	Phenanthrene-d10	17.351

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	98
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5			Octadecanoic acid	284	C18H36O2	000057-11-4	93



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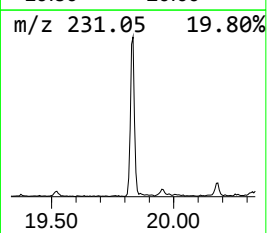
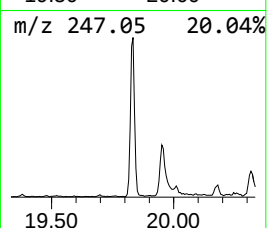
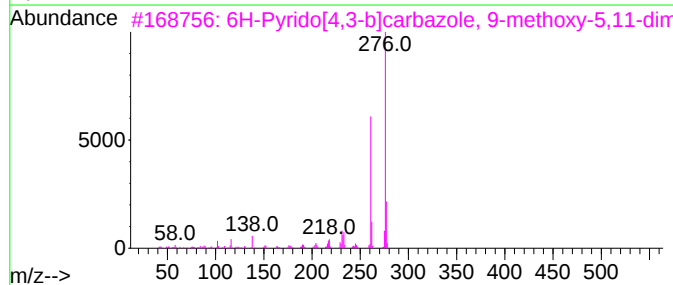
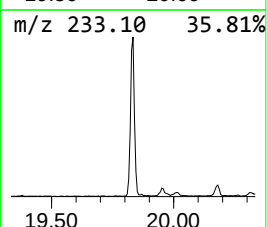
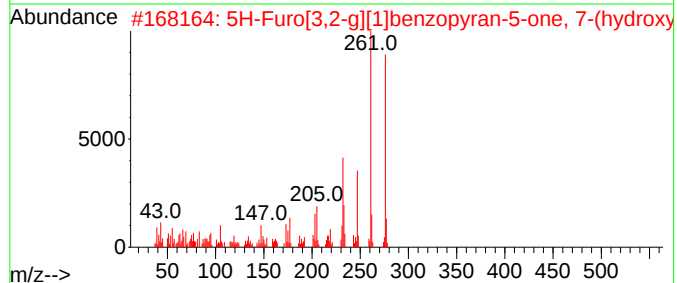
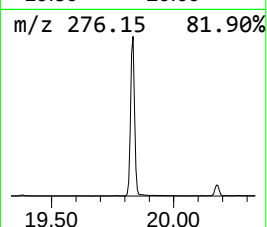
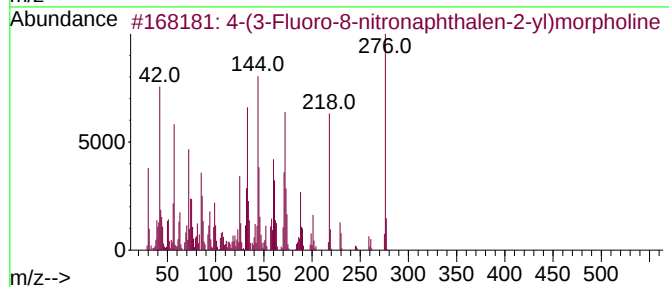
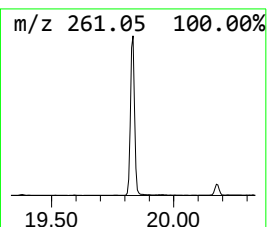
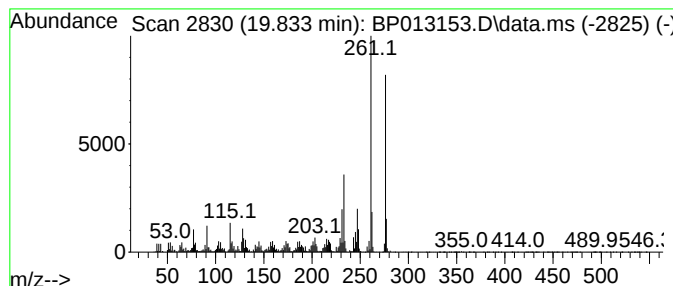
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4-(3-Fluoro-8-nitronaphthal... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.833	7.63 ng/ul	2304690	Chrysene-d12	21.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(3-Fluoro-8-nitronaphthalen-2-...	276	C14H13FN2O3	1000409-37-1	92		
2	5H-Furo[3,2-g][1]benzopyran-5-on...	276	C14H12O6	000668-10-0	74		
3	6H-Pyrido[4,3-b]carbazole, 9-met...	276	C18H16N2O	010371-86-5	72		
4	5,6,7,8-Tetrahydrothieno[2,3-b]q...	276	C14H20N2SSi	1000496-40-4	70		
5	(1H)Pyrrole, 3,4-dimethyl-5-meth...	276	C15H20N2OS	1000197-22-6	64		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013153.D
Acq On : 20 Dec 2022 07:24
Operator : CG/JU
Sample : N6003-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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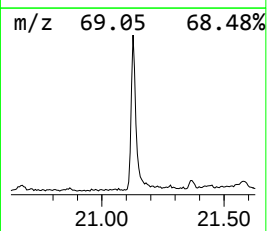
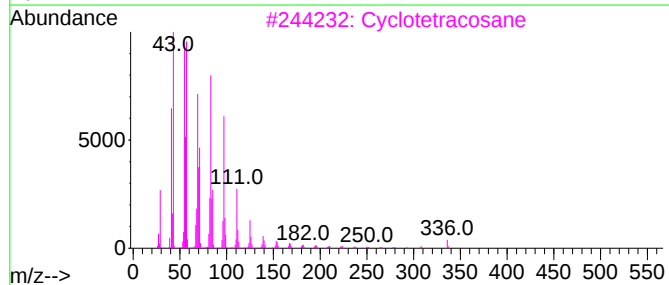
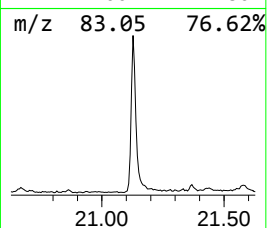
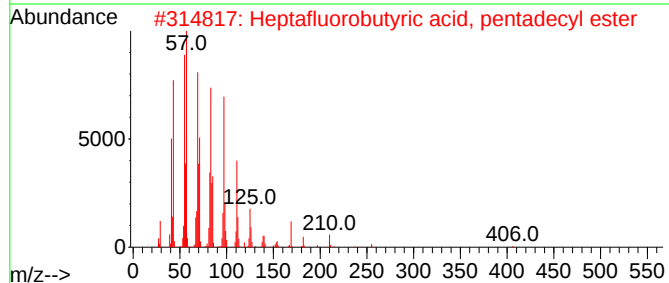
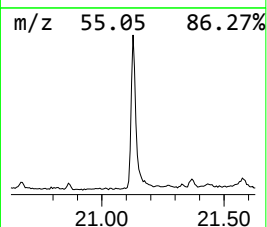
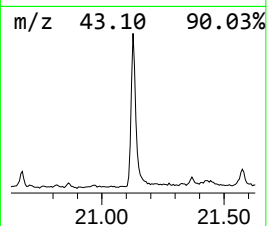
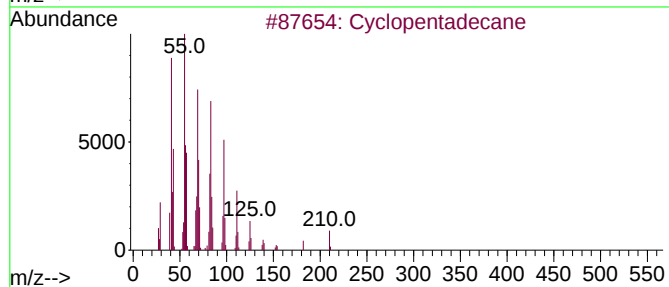
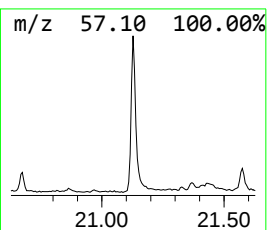
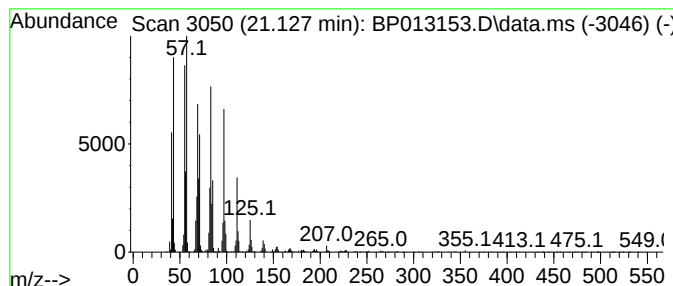
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Cyclic21.128 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	6.33 ng/ul	1913490	Chrysene-d12	21.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			Cyclotetracosane	336	C24H48	000297-03-0	94
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
5			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013153.D
Acq On : 20 Dec 2022 07:24
Operator : CG/JU
Sample : N6003-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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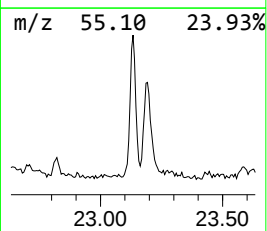
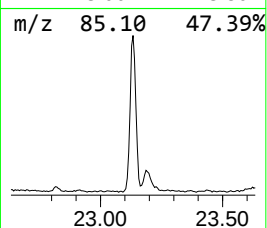
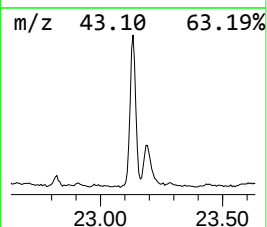
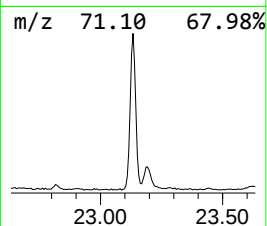
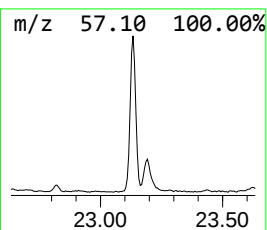
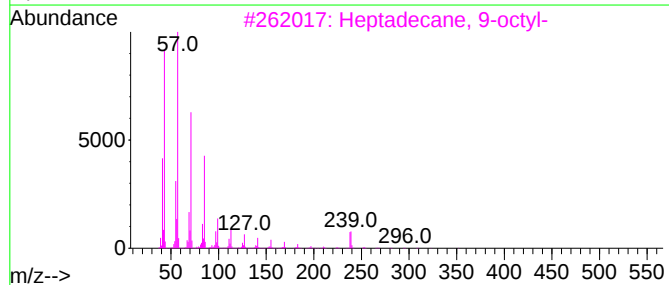
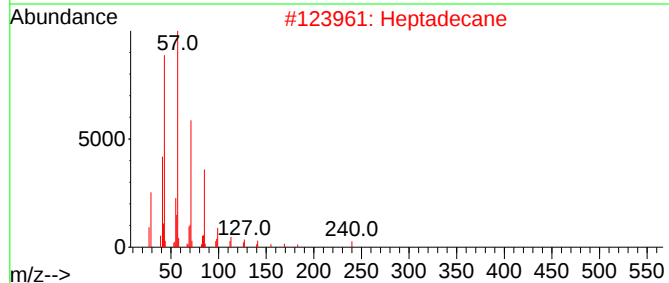
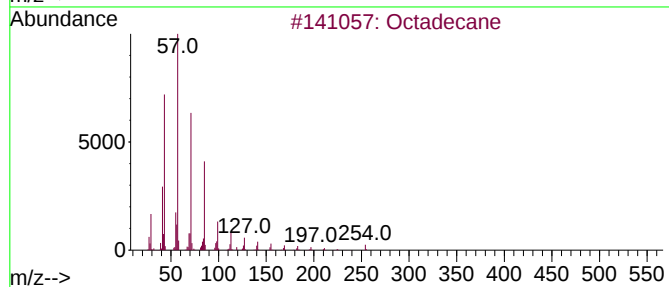
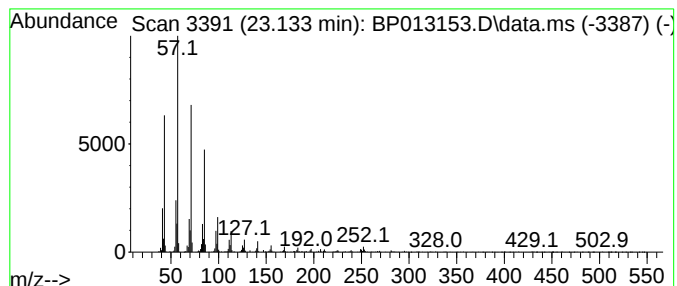
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.133	3.12 ng/ul	1135130	Perylene-d12	23.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	95
2			Heptadecane	240	C17H36	000629-78-7	94
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
4			Hexacosane	366	C26H54	000630-01-3	93
5			Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013153.D
Acq On : 20 Dec 2022 07:24
Operator : CG/JU
Sample : N6003-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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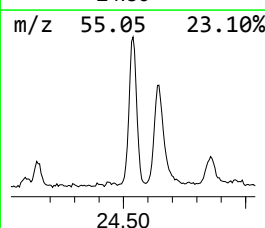
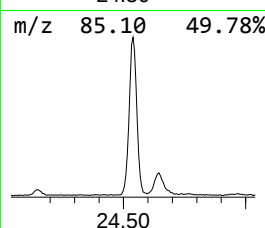
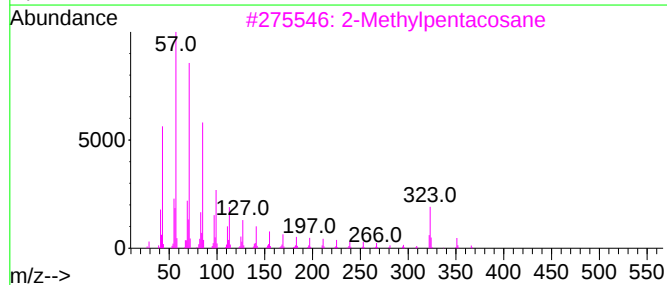
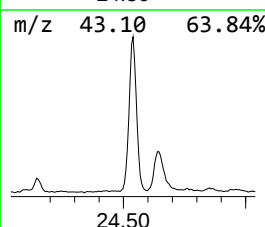
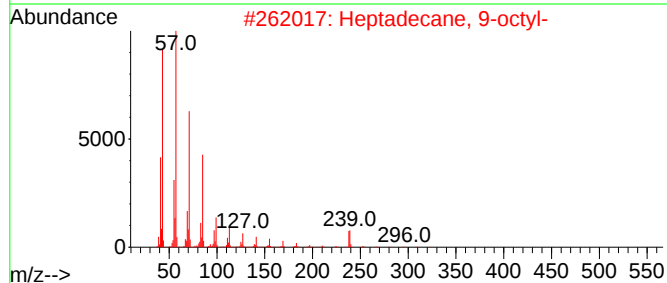
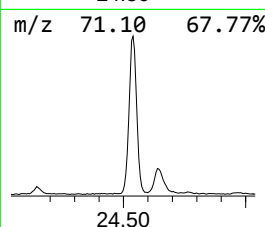
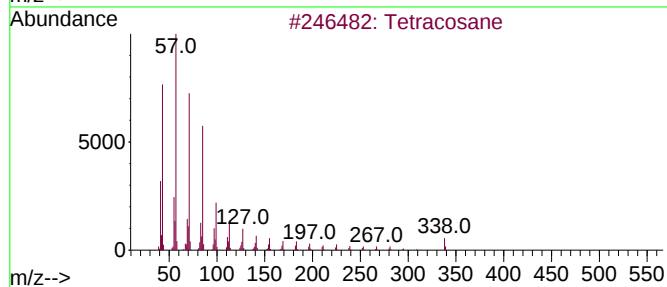
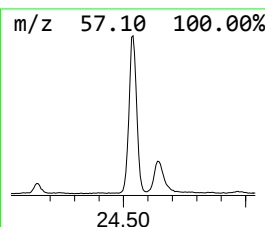
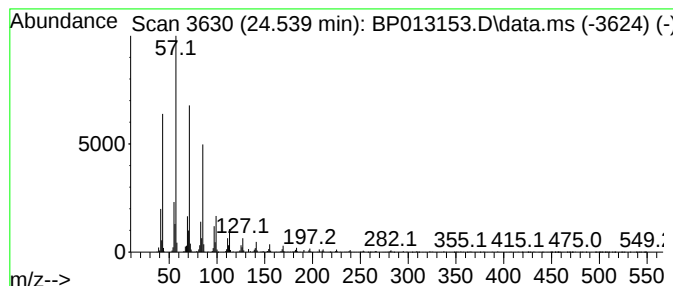
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.539	9.20 ng/ul	3349310	Perylene-d12	23.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	98
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
3			2-Methylpentacosane	366	C26H54	000629-87-8	94
4			Eicosane	282	C20H42	000112-95-8	93
5			Docosane, 7-hexyl-	394	C28H58	055373-86-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013153.D
Acq On : 20 Dec 2022 07:24
Operator : CG/JU
Sample : N6003-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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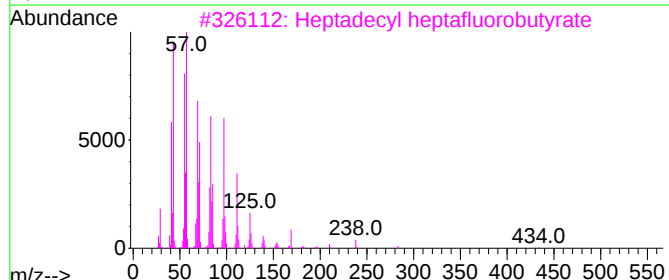
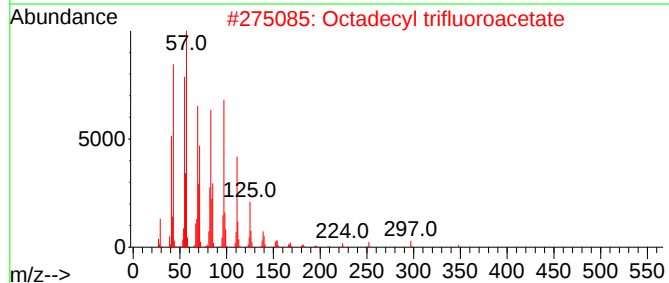
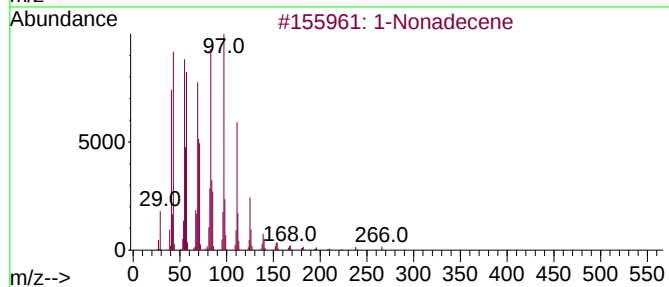
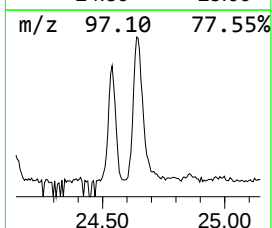
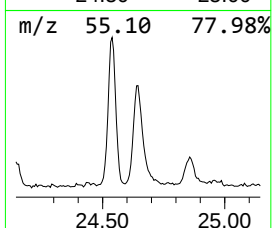
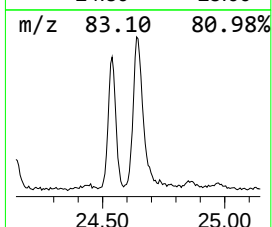
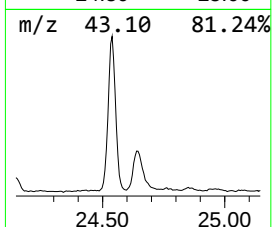
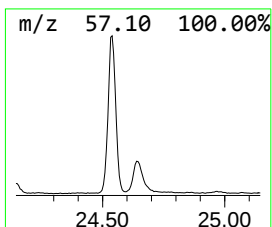
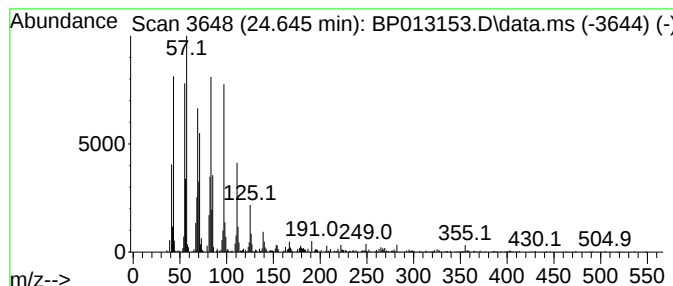
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.645	4.19 ng/ul	1524790	Perylene-d12	23.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	97
2	Octadecyl trifluoroacetate			366	C20H37F3O2	079392-43-1	94
3	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	94
4	n-Tetracosanol-1			354	C24H50O	000506-51-4	93
5	1-Heptacosanol			396	C27H56O	002004-39-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013153.D
Acq On : 20 Dec 2022 07:24
Operator : CG/JU
Sample : N6003-02
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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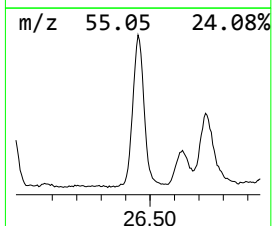
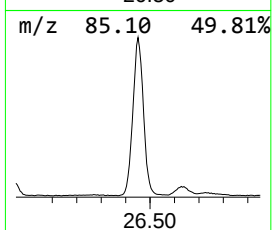
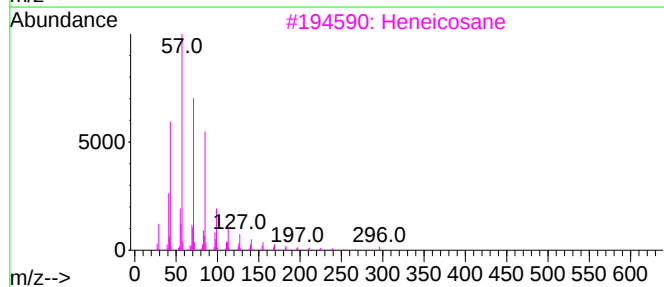
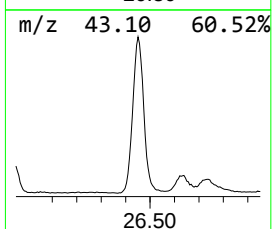
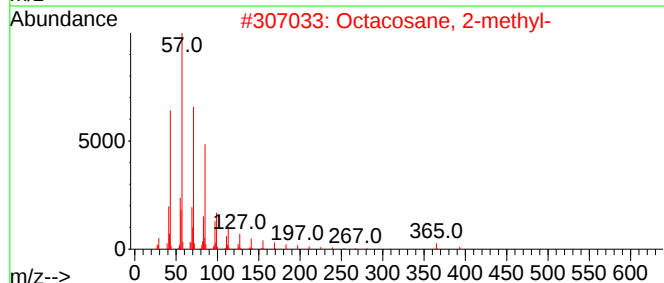
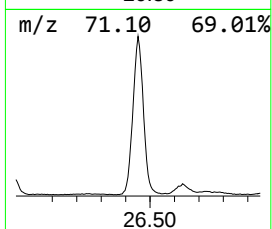
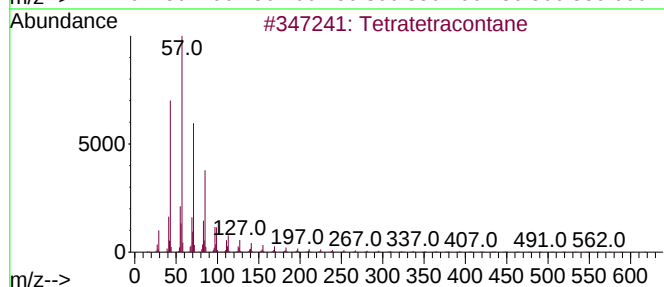
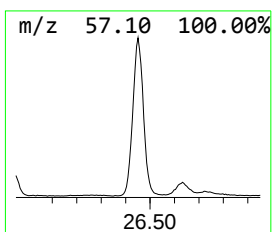
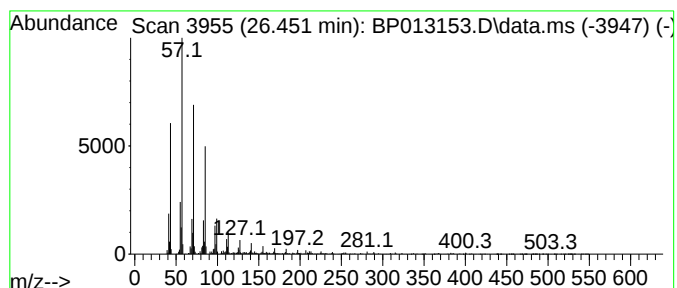
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.451	19.39 ng/ul	7061310	Perylene-d12	23.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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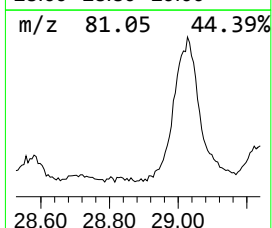
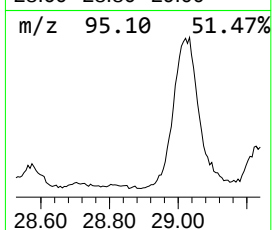
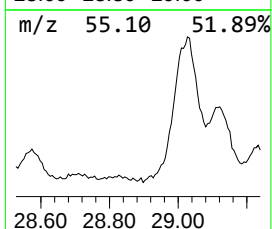
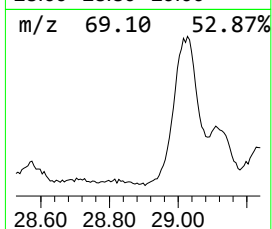
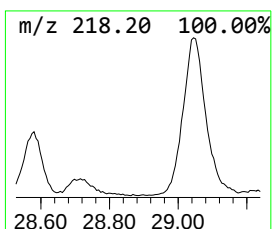
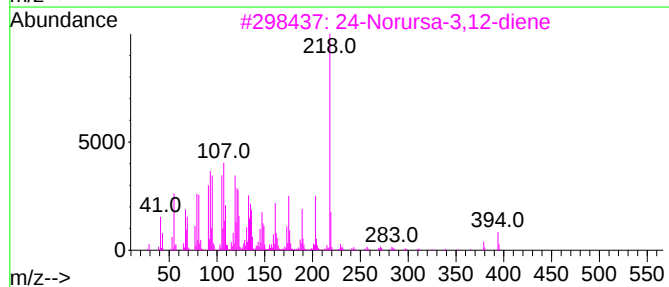
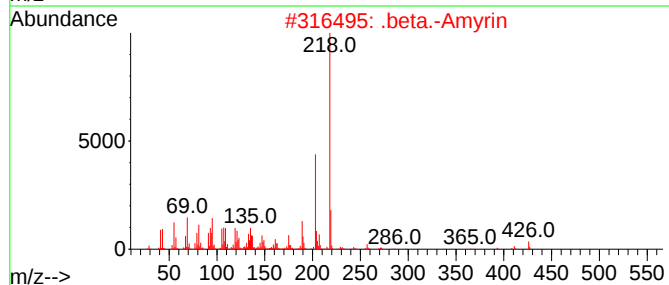
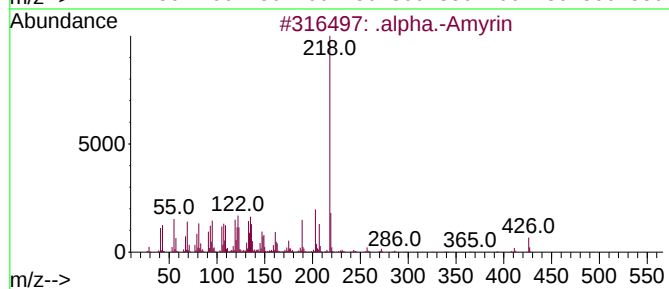
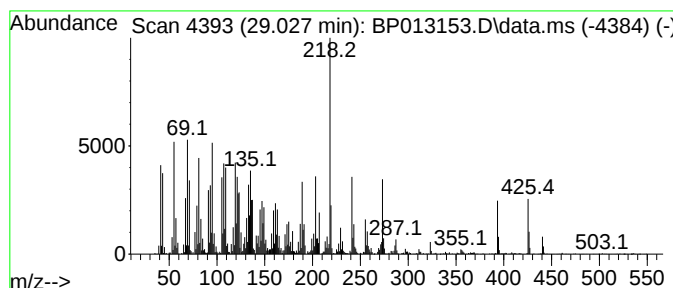
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 .alpha.-Amyrin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
29.027	15.28 ng/ul	5563600	Perylene-d12	23.922	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Amyrin	426	C30H50O	000638-95-9	95
2	.beta.-Amyrin	426	C30H50O	000559-70-6	92
3	24-Norursa-3,12-diene	394	C29H46	201358-25-0	90
4	.beta.-Amyrone	424	C30H48O	000638-97-1	90
5	Lupeol	426	C30H50O	000545-47-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
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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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n-Hexadecanoic ...	18.222	3.7	ng/ul	1072530	4	17.351	5794430	20.0
4-(3-Fluoro-8-n...	19.833	7.6	ng/ul	2304690	5	21.439	6044820	20.0
(DEL) Alkane: C...	21.128	6.3	ng/ul	1913490	5	21.439	6044820	20.0
(DEL) Alkane: S...	23.133	3.1	ng/ul	1135130	6	23.922	7282650	20.0
(DEL) Alkane: S...	24.539	9.2	ng/ul	3349310	6	23.922	7282650	20.0
(DEL) Alkane: S...	24.645	4.2	ng/ul	1524790	6	23.922	7282650	20.0
(DEL) Alkane: S...	26.451	19.4	ng/ul	7061310	6	23.922	7282650	20.0
.alpha.-Amyrin	29.027	15.3	ng/ul	5563600	6	23.922	7282650	20.0