

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
 Data File : BP013211.D
 Acq On : 21 Dec 2022 16:55
 Operator : CG/JU
 Sample : N6014-07
 Misc :
 ALS Vial : 93 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DBXR8

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: BP013211.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	21	25	37	rVB	185826	246937	1.96%	0.156%
2	3.764	94	98	114	rBV	2355981	3393081	26.97%	2.149%
3	3.993	135	137	141	rVB4	24361	28046	0.22%	0.018%
4	4.093	150	154	159	rVB	41035	54679	0.43%	0.035%
5	5.040	310	315	321	rBV	142472	203570	1.62%	0.129%
6	5.281	352	356	363	rVB3	15448	27329	0.22%	0.017%
7	6.934	630	637	641	rBV8	10940	22271	0.18%	0.014%
8	7.111	659	667	682	rBV	2723305	4253891	33.81%	2.694%
9	7.275	689	695	706	rVB	2172512	3375432	26.83%	2.138%
10	7.481	721	730	739	rBV	2752229	4334051	34.45%	2.745%
11	7.952	803	810	818	rBV	1976334	3067704	24.38%	1.943%
12	8.011	818	820	826	rVB6	13678	18755	0.15%	0.012%
13	8.658	923	930	940	rBV	3070138	4892107	38.89%	3.098%
14	9.052	991	997	1001	rBV9	10862	16947	0.13%	0.011%
15	9.116	1001	1008	1018	rBV	2546313	4144982	32.95%	2.625%
16	9.275	1030	1035	1041	rVB6	24652	37971	0.30%	0.024%
17	9.522	1070	1077	1086	rVB	48115	88004	0.70%	0.056%
18	9.846	1123	1132	1145	rBV	2146344	3568554	28.37%	2.260%
19	10.069	1166	1170	1176	rVB9	8940	20484	0.16%	0.013%
20	10.381	1216	1223	1242	rVV	3331151	5468165	43.46%	3.463%
21	10.546	1248	1251	1254	rVB5	10007	14546	0.12%	0.009%
22	10.763	1279	1288	1296	rBV	2627877	4354639	34.61%	2.758%
23	10.905	1304	1312	1328	rBV	2464863	4401876	34.99%	2.788%
24	11.122	1345	1349	1355	rVV8	7334	14783	0.12%	0.009%
25	11.169	1355	1357	1362	rVB6	8421	13770	0.11%	0.009%
26	11.234	1364	1368	1372	rVB7	7634	13053	0.10%	0.008%
27	11.546	1415	1421	1429	rBV7	11193	20186	0.16%	0.013%
28	12.175	1523	1528	1532	rBV3	16591	24546	0.20%	0.016%
29	12.257	1536	1542	1544	rBV7	8186	12691	0.10%	0.008%
30	12.346	1552	1557	1564	rVB	55380	84930	0.68%	0.054%
31	12.563	1586	1594	1598	rBV10	9168	19630	0.16%	0.012%
32	13.122	1683	1689	1691	rVB7	8942	13160	0.10%	0.008%
33	13.193	1696	1701	1707	rVB10	7485	13099	0.10%	0.008%
34	13.322	1718	1723	1727	rBV8	7753	14342	0.11%	0.009%
35	13.404	1727	1737	1745	rVB3	40472	75481	0.60%	0.048%
36	13.546	1757	1761	1769	rVB3	66470	103905	0.83%	0.066%

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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
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37	13.757	1793	1797	1802	rBV8	12996	20333	0.16%	0.013%
38	13.910	1819	1823	1828	rBV8	8013	13822	0.11%	0.009%
39	13.998	1830	1838	1847	rBV	5133319	6898116	54.83%	4.369%
40	14.110	1854	1857	1861	rVB6	11131	14470	0.12%	0.009%
41	14.234	1872	1878	1880	rBV6	8715	13897	0.11%	0.009%
42	14.287	1880	1887	1899	rVV	6059046	8670385	68.92%	5.491%
43	14.475	1916	1919	1924	rVB2	24785	35292	0.28%	0.022%
44	14.546	1924	1931	1934	rBV2	214795	369103	2.93%	0.234%
45	14.593	1934	1939	1949	rVB	3590454	5270682	41.90%	3.338%
46	14.787	1966	1972	1991	rBV	1424295	2342133	18.62%	1.483%
47	14.998	2003	2008	2015	rVB7	45089	76914	0.61%	0.049%
48	15.257	2049	2052	2055	rVB5	10422	15759	0.13%	0.010%
49	15.369	2068	2071	2075	rBV6	10234	14342	0.11%	0.009%
50	15.428	2078	2081	2084	rVB5	12428	17172	0.14%	0.011%
51	15.587	2101	2108	2122	rBV	7346479	10130300	80.52%	6.416%
52	15.704	2122	2128	2140	rVV	1658615	2254384	17.92%	1.428%
53	15.822	2144	2148	2156	rVB2	31332	57186	0.45%	0.036%
54	15.951	2165	2170	2174	rBV	80247	110922	0.88%	0.070%
55	16.157	2202	2205	2212	rVB9	11857	19262	0.15%	0.012%
56	16.292	2225	2228	2230	rVV4	17055	20577	0.16%	0.013%
57	16.345	2233	2237	2247	rVB2	48999	91533	0.73%	0.058%
58	16.445	2250	2254	2258	rVV7	9954	20260	0.16%	0.013%
59	16.734	2299	2303	2309	rVB8	28752	41709	0.33%	0.026%
60	17.092	2362	2364	2368	rVB5	11242	13336	0.11%	0.008%
61	17.134	2368	2371	2374	rBV5	10822	19068	0.15%	0.012%
62	17.228	2383	2387	2395	rBV7	44793	83359	0.66%	0.053%
63	17.298	2395	2399	2401	rBV3	28471	31937	0.25%	0.020%
64	17.351	2401	2408	2413	rBV	3446742	5073951	40.33%	3.214%
65	17.445	2418	2424	2436	rVV	6025649	8999765	71.54%	5.700%
66	17.563	2442	2444	2447	rVB	35213	33505	0.27%	0.021%
67	17.622	2452	2454	2460	rBV7	14355	27612	0.22%	0.017%
68	17.704	2464	2468	2470	rBV5	33217	46860	0.37%	0.030%
69	17.869	2492	2496	2501	rVB6	17832	30932	0.25%	0.020%
70	18.004	2516	2519	2523	rVB6	17959	23641	0.19%	0.015%
71	18.104	2533	2536	2541	rVB4	30457	42399	0.34%	0.027%
72	18.163	2542	2546	2551	rBV2	84022	121648	0.97%	0.077%
73	18.222	2551	2556	2572	rBV	730189	1200591	9.54%	0.760%
74	18.504	2601	2604	2608	rBV4	27077	38452	0.31%	0.024%
75	18.628	2621	2625	2630	rBV	224492	253742	2.02%	0.161%
76	19.204	2720	2723	2726	rBV2	39968	54027	0.43%	0.034%

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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

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 Title : SVOA CALIBRATION

77	19.257	2729	2732	2736	rVB2	79367	100501	0.80%	0.064%
78	19.351	2738	2748	2756	rBV2	311902	723990	5.75%	0.459%
79	19.451	2761	2765	2771	rBV	206855	316660	2.52%	0.201%
80	19.681	2798	2804	2816	rBV	7645134	10352727	82.29%	6.557%
81	19.828	2826	2829	2832	rBV2	82637	90315	0.72%	0.057%
82	21.128	3046	3050	3060	rBV3	874300	1399774	11.13%	0.887%
83	21.433	3096	3102	3107	rBV	4100783	5636042	44.80%	3.570%
84	23.127	3386	3390	3407	rVB2	1011579	2459136	19.55%	1.557%
85	23.757	3490	3497	3512	rVB	5903833	12580653	100.00%	7.968%
86	23.916	3517	3524	3531	rBV2	2918224	5897889	46.88%	3.735%
87	24.421	3603	3610	3621	rVB	5680430	12446540	98.93%	7.883%
88	24.533	3624	3629	3638	rVB	859752	1841499	14.64%	1.166%
89	24.716	3656	3660	3673	rVB5	791951	1716468	13.64%	1.087%
90	26.439	3948	3953	3968	rVB3	1051825	3259447	25.91%	2.064%

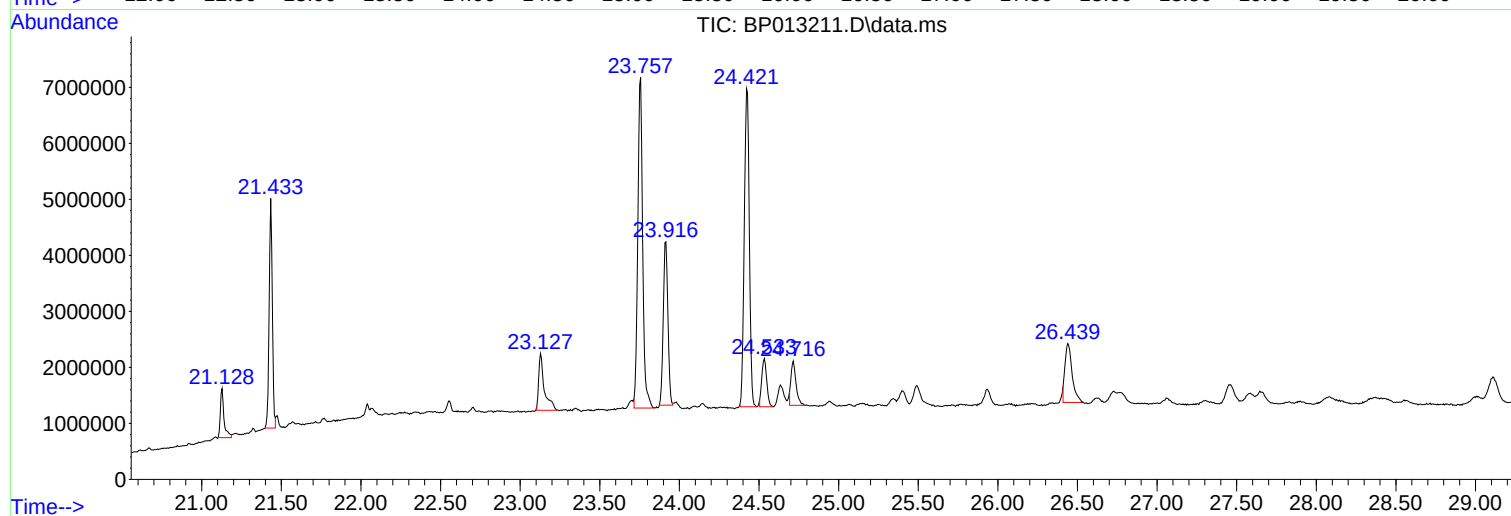
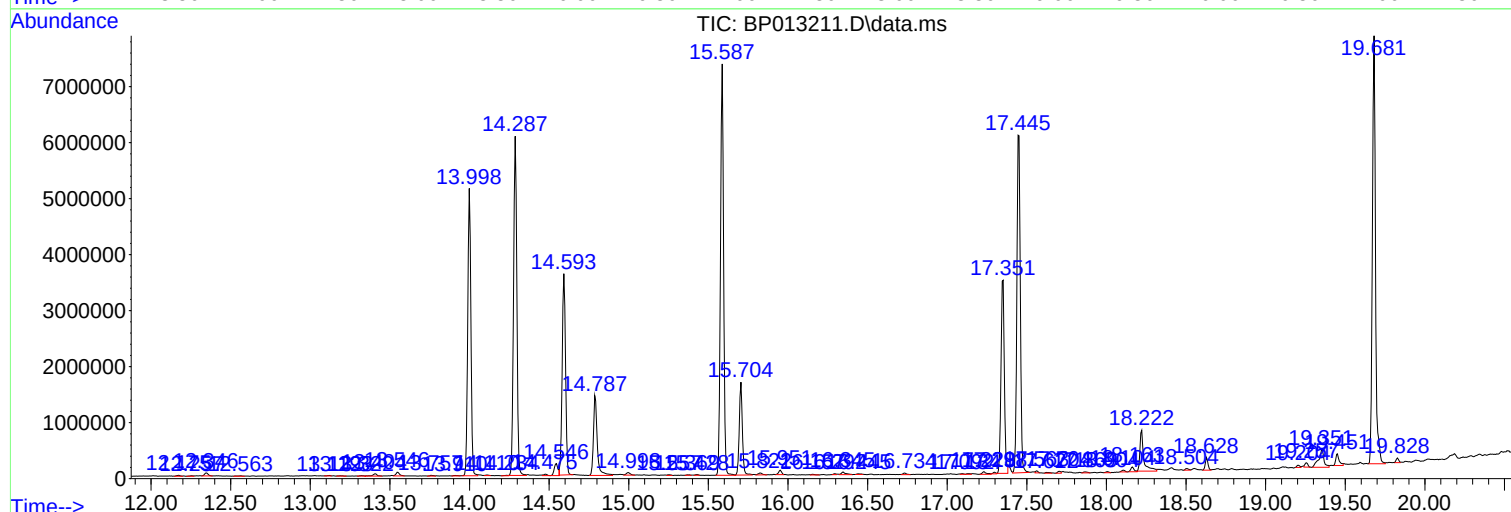
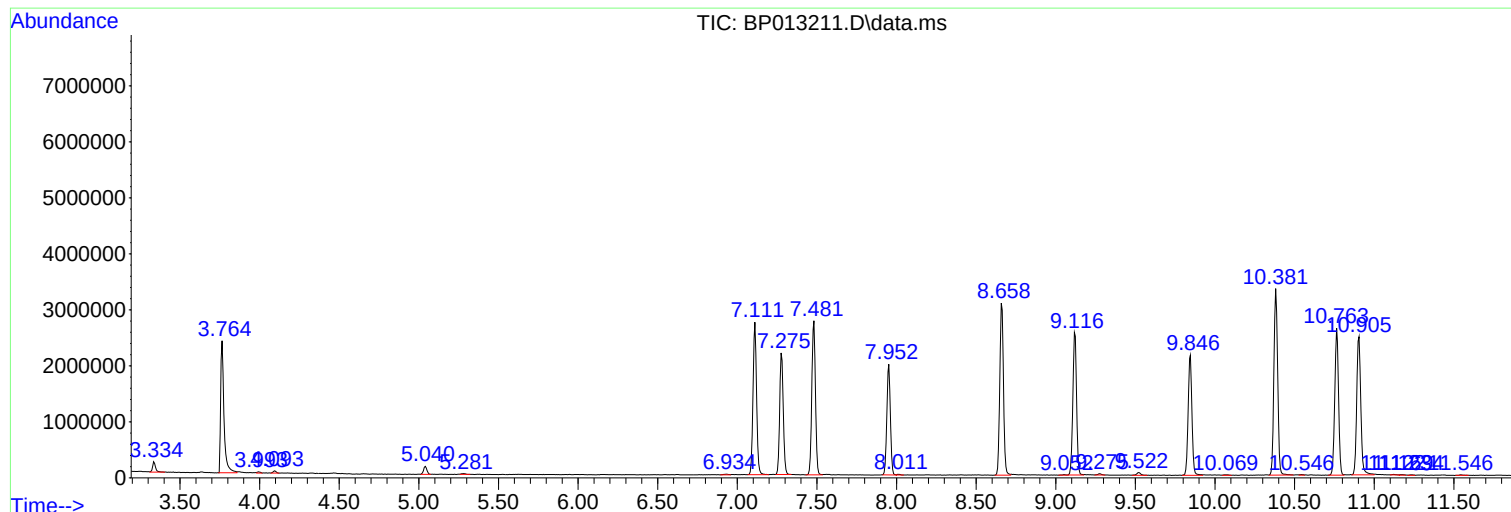
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



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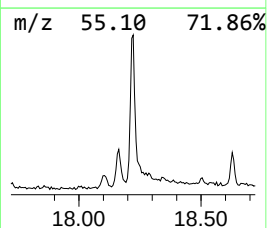
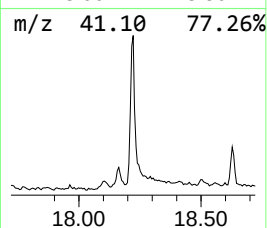
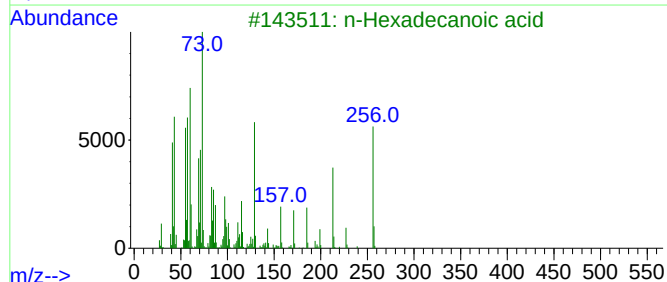
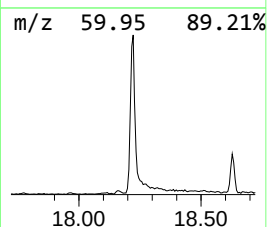
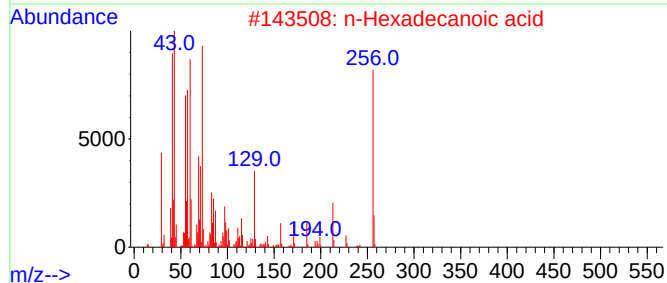
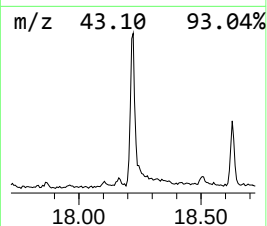
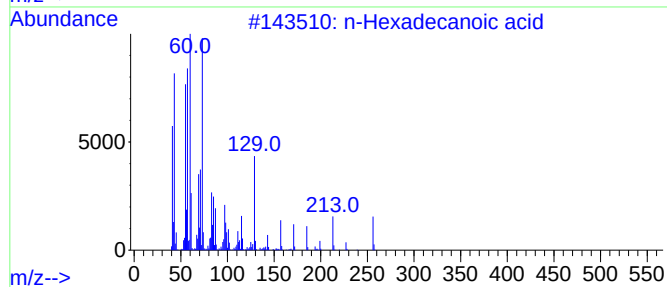
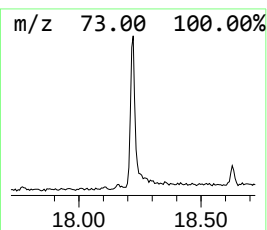
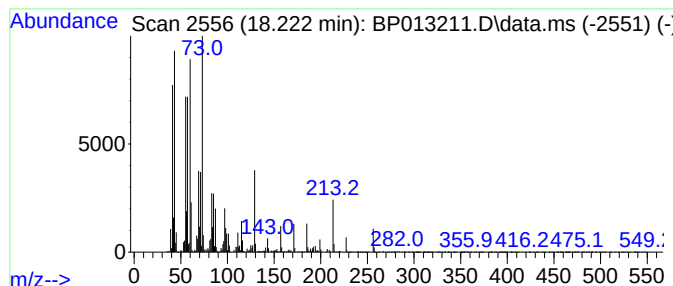
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	4.73 ng/ul	1200590	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	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93



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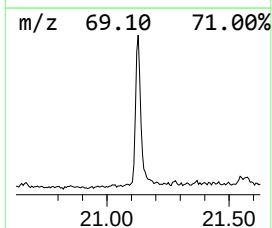
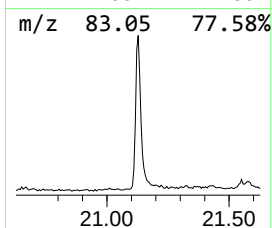
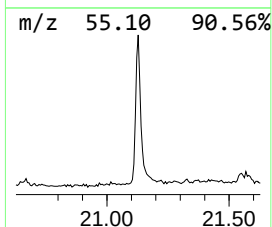
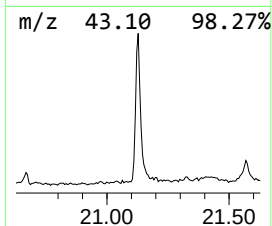
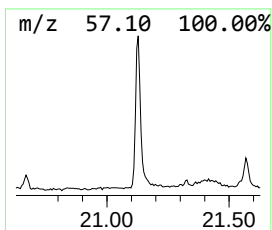
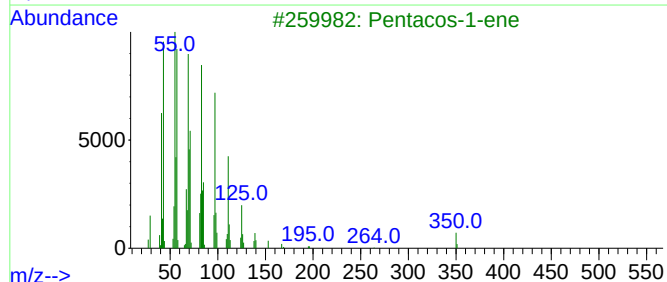
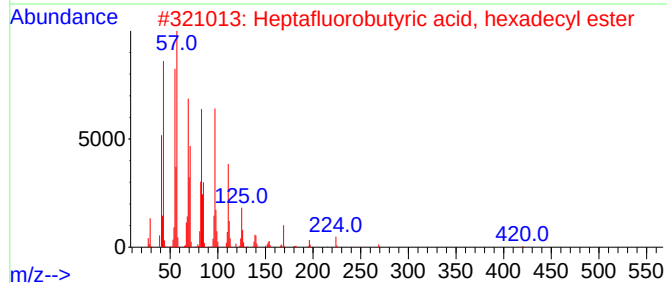
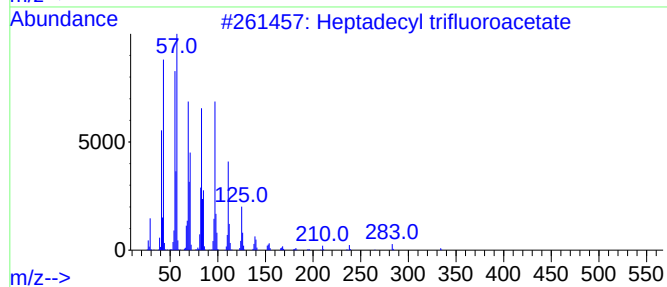
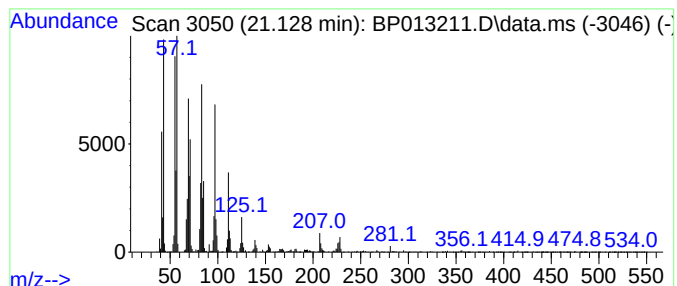
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Heptadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	4.97 ng/ul	1399770	Chrysene-d12	21.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5			Octacosanol	410	C28H58O	000557-61-9	94



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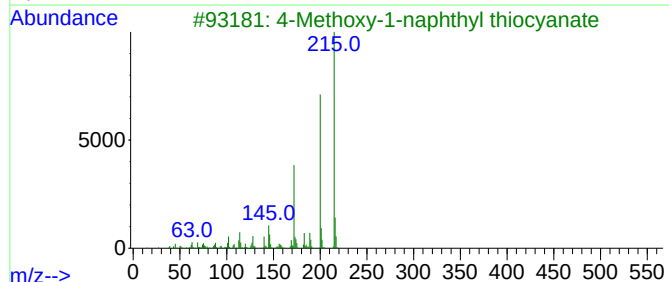
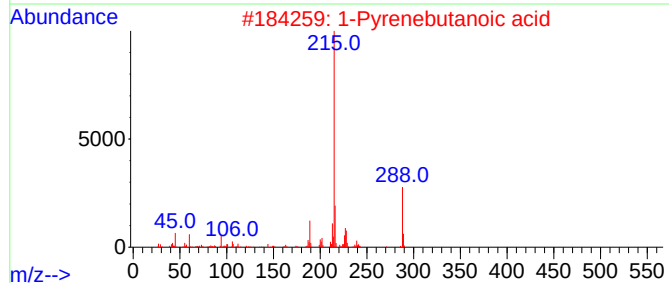
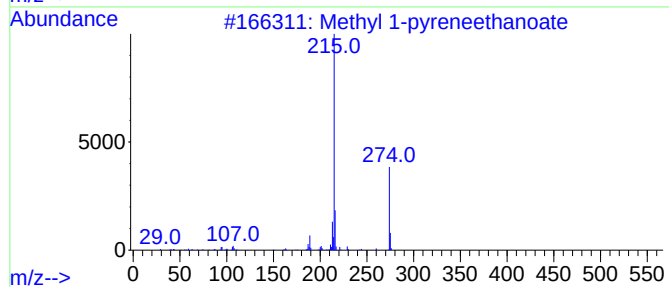
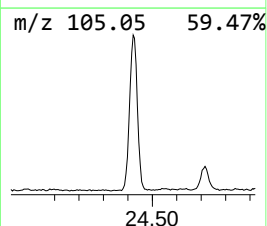
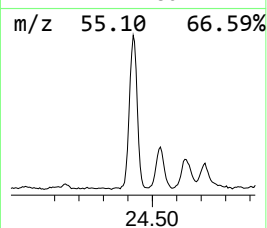
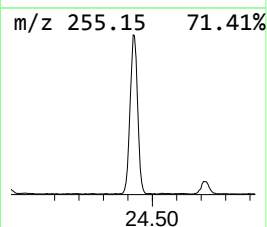
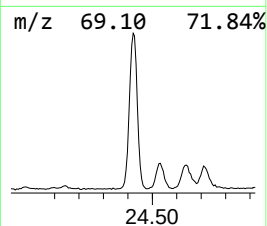
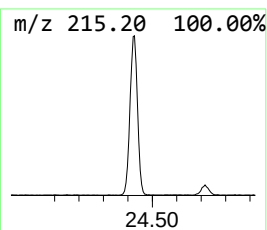
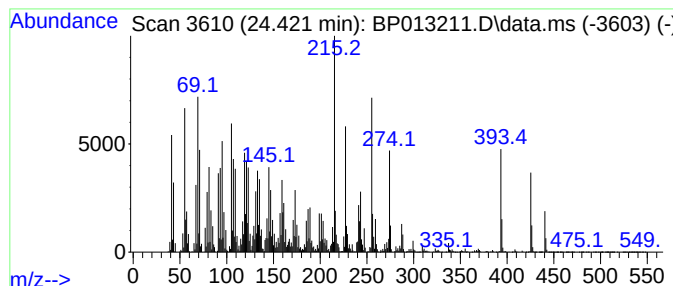
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.421	42.21 ng/ul	12446500	Perylene-d12	23.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 1-pyreneethanoate	274	C19H14O2	073654-19-0	42
2			1-Pyrenebutanoic acid	288	C20H16O2	003443-45-6	20
3			4-Methoxy-1-naphthyl thiocyanate	215	C12H9NOS	066231-77-4	20
4			5-Chloro-2-methoxyphenylamine, N...	215	C9H10ClNO3	1000343-98-2	18
5			4-(1H-Indol-3-yl)-1,3-thiazol-2-...	215	C11H9N3S	022258-56-6	18



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Instrument :
BNA_P
ClientSampleId :
DBXR8

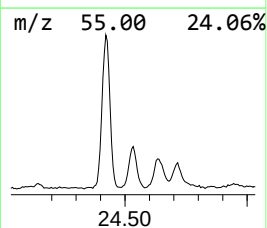
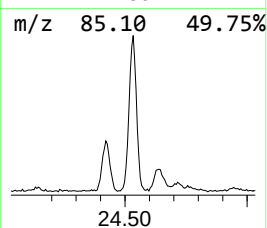
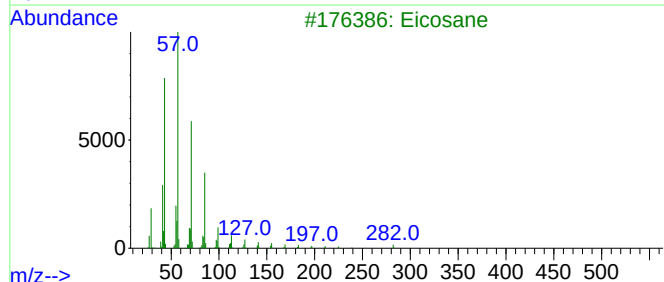
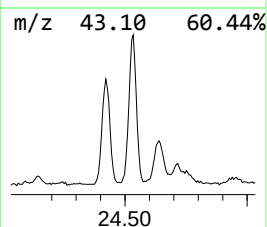
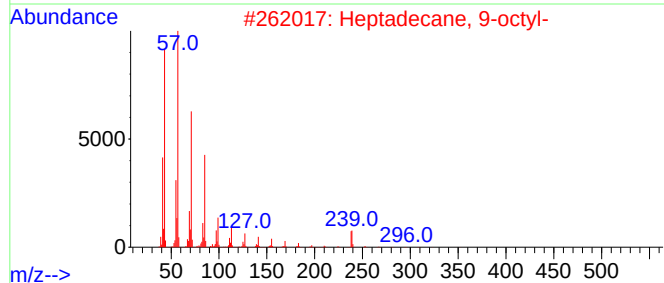
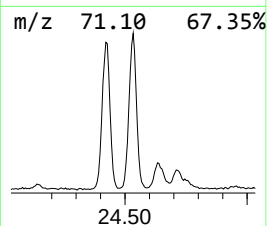
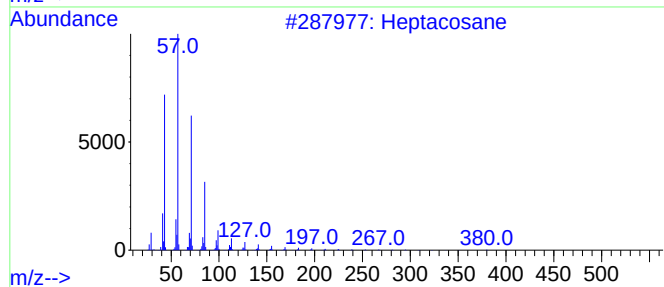
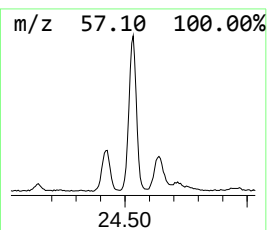
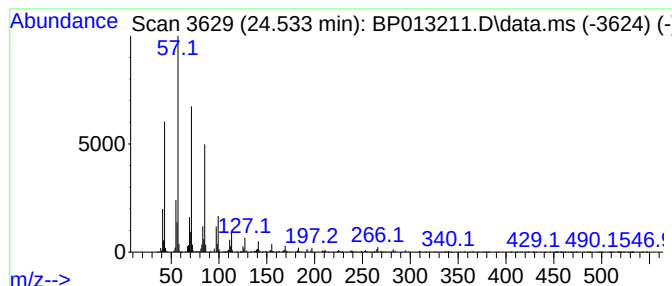
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.533	6.24 ng/ul	1841500	Perylene-d12	23.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	95
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
3			Eicosane	282	C20H42	000112-95-8	92
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
5			Eicosane, 10-methyl-	296	C21H44	054833-23-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013211.D
Acq On : 21 Dec 2022 16:55
Operator : CG/JU
Sample : N6014-07
Misc :
ALS Vial : 93 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXR8

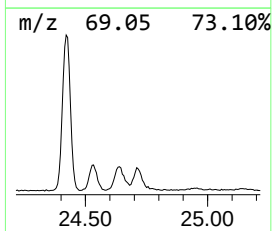
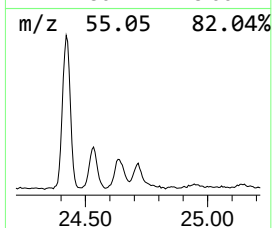
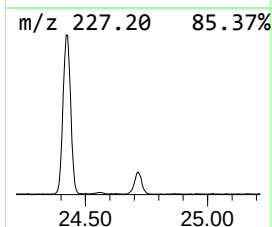
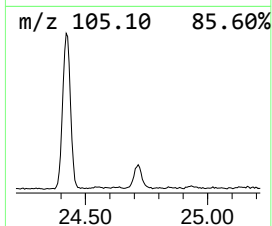
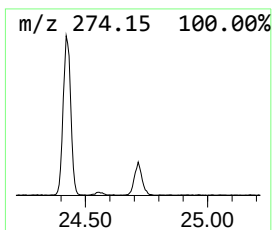
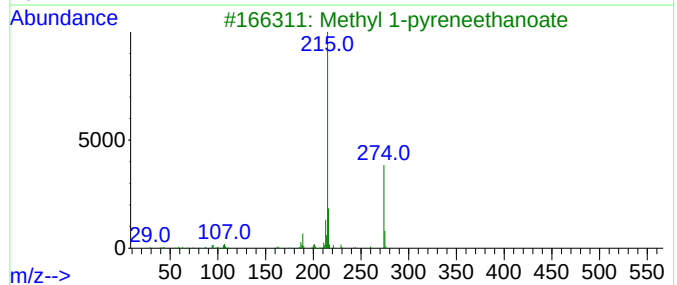
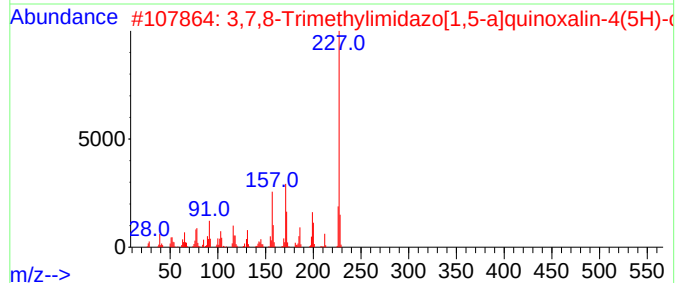
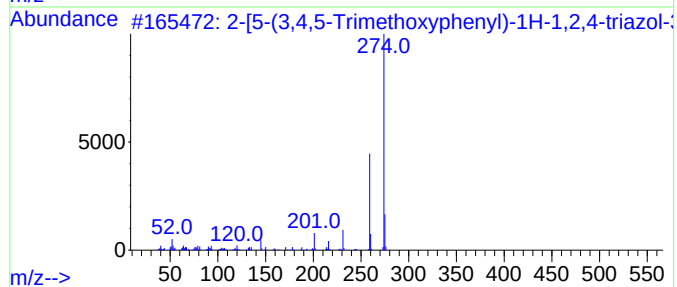
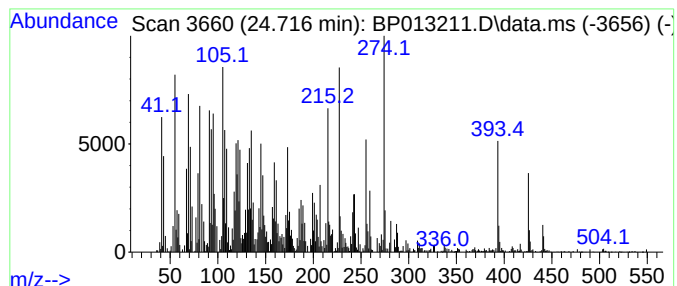
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 2-[5-(3,4,5-Trimethoxyphenyl)-1H... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.716	5.82 ng/ul	1716470	Perylene-d12	23.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2	-[5-(3,4,5-Trimethoxyphenyl)-1H...	274	C13H14N4O3	1000435-80-6	53	
2	3,7,8-Trimethylimidazo[1,5-a]qui...	227	C13H13N3O	1404093-54-4	46		
3	Methyl 1-pyreneethanoate	274	C19H14O2	073654-19-0	38		
4	N,4-Dicyclopentenyl-2-methoxyani...	255	C17H21NO	1000441-76-4	35		
5	Estr-5(10)-en-3-one, 17.beta.-hy...	274	C18H26O2	001089-78-7	30		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013211.D
Acq On : 21 Dec 2022 16:55
Operator : CG/JU
Sample : N6014-07
Misc :
ALS Vial : 93 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXR8

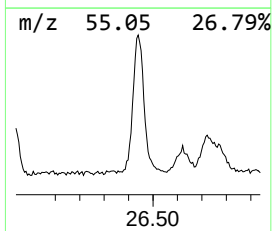
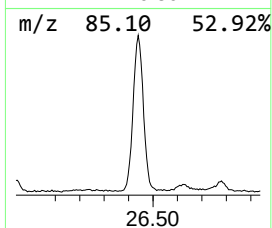
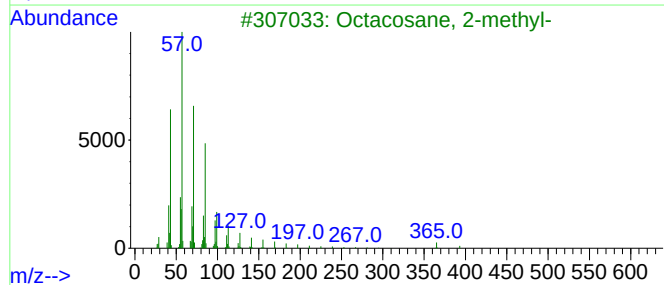
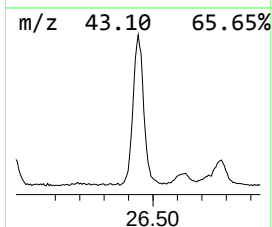
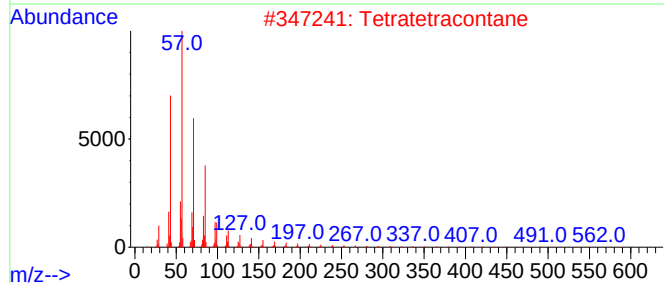
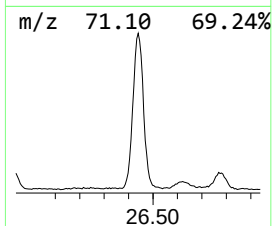
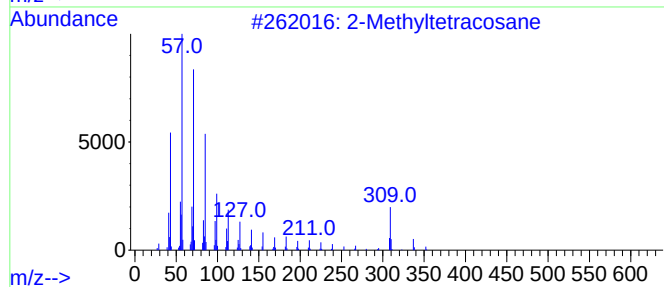
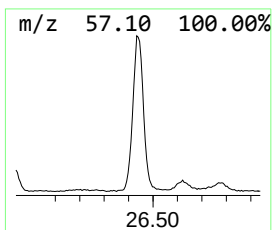
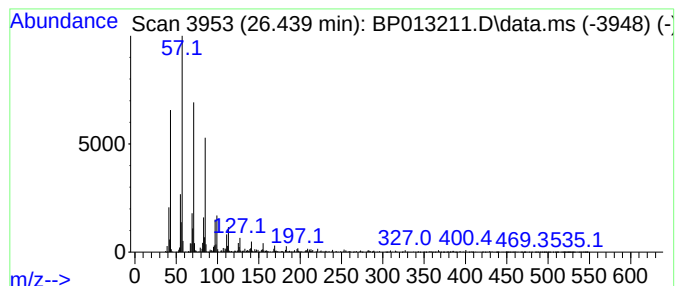
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.439	11.05 ng/ul	3259450	Perylene-d12	23.916

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyltetracosane	352	C25H52	001560-78-7	93	
2	Tetratetracontane	619	C44H90	007098-22-8	91	
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90	
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90	
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013211.D
Acq On : 21 Dec 2022 16:55
Operator : CG/JU
Sample : N6014-07
Misc :
ALS Vial : 93 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXR8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
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
n-Hexadecanoic ...	18.222	4.7	ng/ul	1200590	4	17.351	5073950	20.0
Heptadecyl trif...	21.128	5.0	ng/ul	1399770	5	21.433	5636040	20.0
unknown-01	24.421	42.2	ng/ul	12446500	6	23.916	5897890	20.0
(DEL) Alkane: S...	24.533	6.2	ng/ul	1841500	6	23.916	5897890	20.0
2-[5-(3,4,5-Tri...	24.716	5.8	ng/ul	1716470	6	23.916	5897890	20.0
(DEL) Alkane: S...	26.439	11.1	ng/ul	3259450	6	23.916	5897890	20.0