

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
 Data File : BP018781.D
 Acq On : 12 Dec 2023 23:06
 Operator : MA/JU
 Sample : 05646-04
 Misc :
 ALS Vial : 60 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0AT8

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-BP120123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP018781.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.264	26	30	38	rVB	31979	47235	1.15%	0.105%
2	3.546	75	78	84	rBV	52655	76234	1.86%	0.170%
3	3.687	99	102	112	rBV	101164	153643	3.74%	0.342%
4	3.793	116	120	125	rBV	24394	32393	0.79%	0.072%
5	3.887	130	136	137	rVV5	10843	15167	0.37%	0.034%
6	3.917	137	141	145	rVB2	26802	40134	0.98%	0.089%
7	4.011	153	157	162	rVB2	11516	18416	0.45%	0.041%
8	4.528	241	245	248	rVB6	4011	6139	0.15%	0.014%
9	4.575	248	253	259	rBV8	9346	18236	0.44%	0.041%
10	4.740	279	281	288	rVB6	4109	6484	0.16%	0.014%
11	4.934	309	314	323	rVB2	33767	61068	1.49%	0.136%
12	5.146	342	350	357	rBV	226870	337361	8.21%	0.750%
13	5.552	414	419	426	rVB8	6370	13250	0.32%	0.029%
14	5.822	461	465	470	rBV4	6476	10896	0.27%	0.024%
15	5.928	479	483	486	rVB3	6943	9285	0.23%	0.021%
16	6.840	635	638	643	rVB7	5708	8833	0.21%	0.020%
17	7.005	657	666	677	rVB	503106	923739	22.48%	2.054%
18	7.175	689	695	705	rVB	430572	658897	16.03%	1.465%
19	7.369	722	728	736	rBV	533635	821538	19.99%	1.827%
20	7.452	738	742	748	rBV3	18370	29523	0.72%	0.066%
21	7.722	784	788	794	rBV7	7818	10875	0.26%	0.024%
22	7.840	801	808	818	rBV	645940	1063608	25.88%	2.365%
23	7.911	818	820	827	rVB5	10908	17051	0.41%	0.038%
24	8.081	842	849	851	rBV8	3679	6977	0.17%	0.016%
25	8.299	880	886	891	rVB9	2988	7344	0.18%	0.016%
26	8.546	922	928	937	rBV	504416	819313	19.94%	1.822%
27	8.663	941	948	959	rVV	289143	464542	11.30%	1.033%
28	8.799	966	971	978	rVB3	9600	21251	0.52%	0.047%
29	8.999	997	1005	1015	rBV	495180	786798	19.15%	1.750%
30	9.111	1019	1024	1030	rVB7	4712	8182	0.20%	0.018%
31	9.169	1030	1034	1036	rBV5	5374	7467	0.18%	0.017%
32	9.416	1072	1076	1083	rVB8	6465	12759	0.31%	0.028%
33	9.569	1096	1102	1107	rBV	37526	55893	1.36%	0.124%
34	9.716	1119	1127	1135	rBV	383180	612396	14.90%	1.362%
35	9.881	1145	1155	1161	rBV	59443	118882	2.89%	0.264%
36	9.958	1165	1168	1173	rVB7	6046	8612	0.21%	0.019%

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37	10.081	1181	1189	1195	rVB	31447	54765	1.33%	0.122%
38	10.205	1204	1210	1212	rBV7	3111	6472	0.16%	0.014%
39	10.252	1212	1218	1232	rVV	640207	1051539	25.59%	2.339%
40	10.634	1274	1283	1292	rVB	851047	1408021	34.26%	3.131%
41	10.775	1300	1307	1318	rBV	258453	473223	11.52%	1.052%
42	11.105	1357	1363	1367	rBV9	6945	11850	0.29%	0.026%
43	11.181	1369	1376	1383	rVV8	27294	52977	1.29%	0.118%
44	11.381	1403	1410	1414	rBV	62509	113541	2.76%	0.253%
45	11.422	1414	1417	1429	rVB	23681	47822	1.16%	0.106%
46	11.675	1454	1460	1466	rVB6	6645	13517	0.33%	0.030%
47	11.899	1492	1498	1503	rBV10	3037	6441	0.16%	0.014%
48	11.999	1512	1515	1519	rVB2	9365	13868	0.34%	0.031%
49	12.157	1535	1542	1548	rBV	37047	67706	1.65%	0.151%
50	12.216	1548	1552	1556	rVB3	11988	19941	0.49%	0.044%
51	12.810	1646	1653	1662	rBV4	12851	34555	0.84%	0.077%
52	13.299	1732	1736	1741	rVB4	8822	11790	0.29%	0.026%
53	13.375	1741	1749	1751	rBV3	27133	49652	1.21%	0.110%
54	13.881	1829	1835	1845	rBV	1215797	1689802	41.12%	3.758%
55	14.157	1871	1882	1894	rBV	1245544	1905788	46.38%	4.238%
56	14.469	1927	1935	1944	rBV	1274694	1942055	47.26%	4.319%
57	14.669	1962	1969	1990	rBV	474008	787859	19.17%	1.752%
58	14.822	1990	1995	2001	rVV3	35208	59659	1.45%	0.133%
59	14.887	2002	2006	2013	rVB8	17959	30288	0.74%	0.067%
60	15.269	2064	2071	2072	rBV7	5199	7620	0.19%	0.017%
61	15.281	2072	2073	2078	rVV5	4215	5870	0.14%	0.013%
62	15.457	2097	2103	2110	rBV	1848514	2569143	62.52%	5.714%
63	15.516	2112	2113	2117	rVV4	11624	13687	0.33%	0.030%
64	15.575	2117	2123	2136	rVV	396582	571674	13.91%	1.271%
65	15.698	2141	2144	2151	rVB6	10039	16600	0.40%	0.037%
66	15.910	2177	2180	2185	rVB6	7370	10003	0.24%	0.022%
67	16.516	2278	2283	2285	rBV6	3876	7220	0.18%	0.016%
68	16.616	2296	2300	2305	rBV6	7593	11607	0.28%	0.026%
69	16.681	2308	2311	2312	rBV3	6201	6270	0.15%	0.014%
70	16.751	2318	2323	2330	rVB6	12463	26030	0.63%	0.058%
71	16.981	2355	2362	2368	rBV6	6775	19785	0.48%	0.044%
72	17.216	2395	2402	2408	rBV	1719603	2492227	60.65%	5.543%
73	17.310	2412	2418	2429	rVV	2074402	2876210	69.99%	6.397%
74	17.410	2432	2435	2441	rVB6	21379	31179	0.76%	0.069%
75	17.716	2483	2487	2491	rVB3	21865	26036	0.63%	0.058%
76	17.892	2513	2517	2523	rVB9	12894	17278	0.42%	0.038%

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77	17.981	2527	2532	2538	rBV2	24478	37732	0.92%	0.084%
78	18.104	2548	2553	2564	rBV	300832	440288	10.71%	0.979%
79	18.522	2621	2624	2628	rVB4	22591	26050	0.63%	0.058%
80	18.575	2629	2633	2637	rVB	21456	29872	0.73%	0.066%
81	18.663	2644	2648	2656	rVB	64176	88056	2.14%	0.196%
82	18.881	2681	2685	2689	rBV	62147	81519	1.98%	0.181%
83	18.922	2689	2692	2698	rVB2	25497	29196	0.71%	0.065%
84	19.004	2702	2706	2711	rBV5	25229	40929	1.00%	0.091%
85	19.128	2720	2727	2735	rBV7	80518	202217	4.92%	0.450%
86	19.192	2736	2738	2742	rVB	43810	48420	1.18%	0.108%
87	19.339	2759	2763	2773	rBV	122137	170271	4.14%	0.379%
88	19.551	2793	2799	2805	rBV	2994036	3916876	95.31%	8.711%
89	20.081	2885	2889	2894	rVB	141138	153270	3.73%	0.341%
90	20.563	2969	2971	2974	rVB2	51307	47177	1.15%	0.105%
91	20.728	2994	2999	3003	rBV2	317612	405230	9.86%	0.901%
92	20.910	3027	3030	3035	rBV	174825	209461	5.10%	0.466%
93	21.022	3045	3049	3051	rBV	348181	451898	11.00%	1.005%
94	21.051	3051	3054	3059	rVB	425752	502936	12.24%	1.119%
95	21.304	3091	3097	3103	rBV	2508391	3268472	79.53%	7.269%
96	21.904	3196	3199	3202	rBV	202256	266295	6.48%	0.592%
97	22.945	3371	3376	3381	rBV	416900	663944	16.16%	1.477%
98	23.004	3383	3386	3396	rVB3	176668	400551	9.75%	0.891%
99	23.510	3465	3472	3478	rBV2	2098704	4109504	100.00%	9.140%
100	23.663	3491	3498	3516	rVB	1731884	3501722	85.21%	7.788%

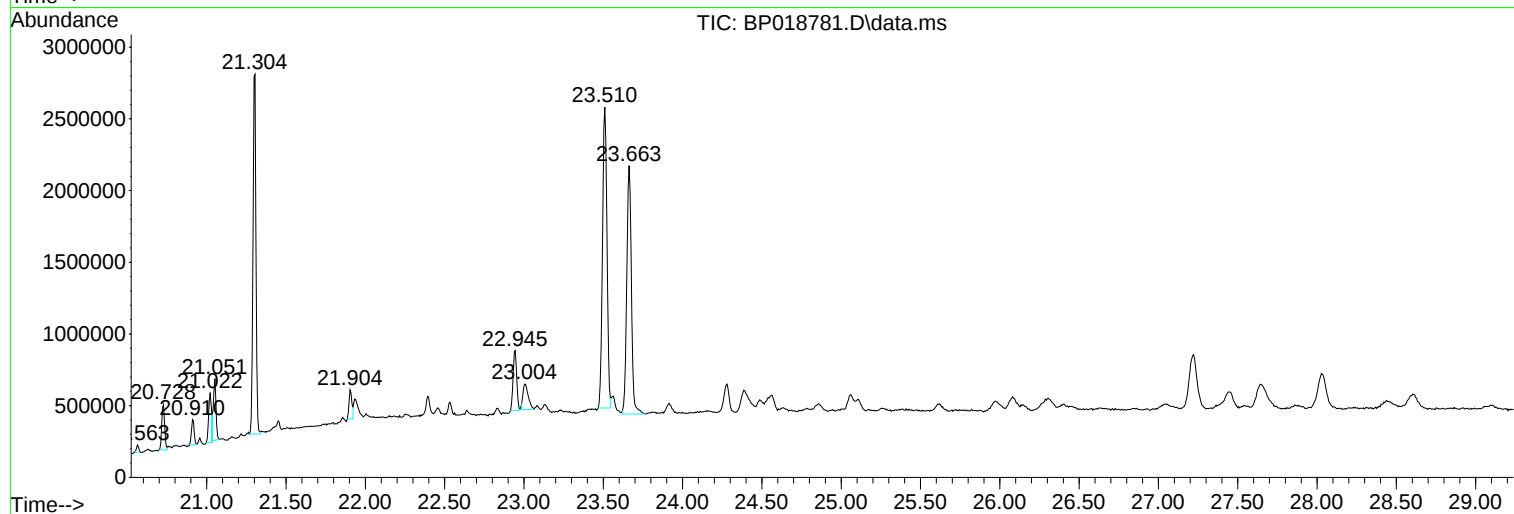
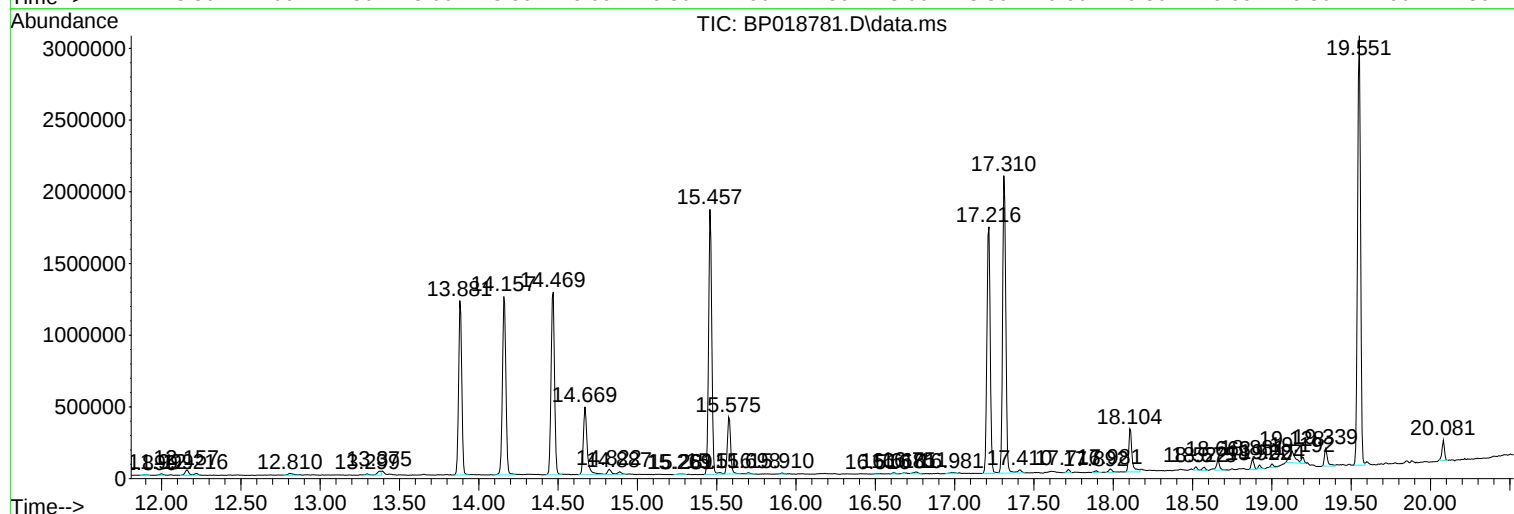
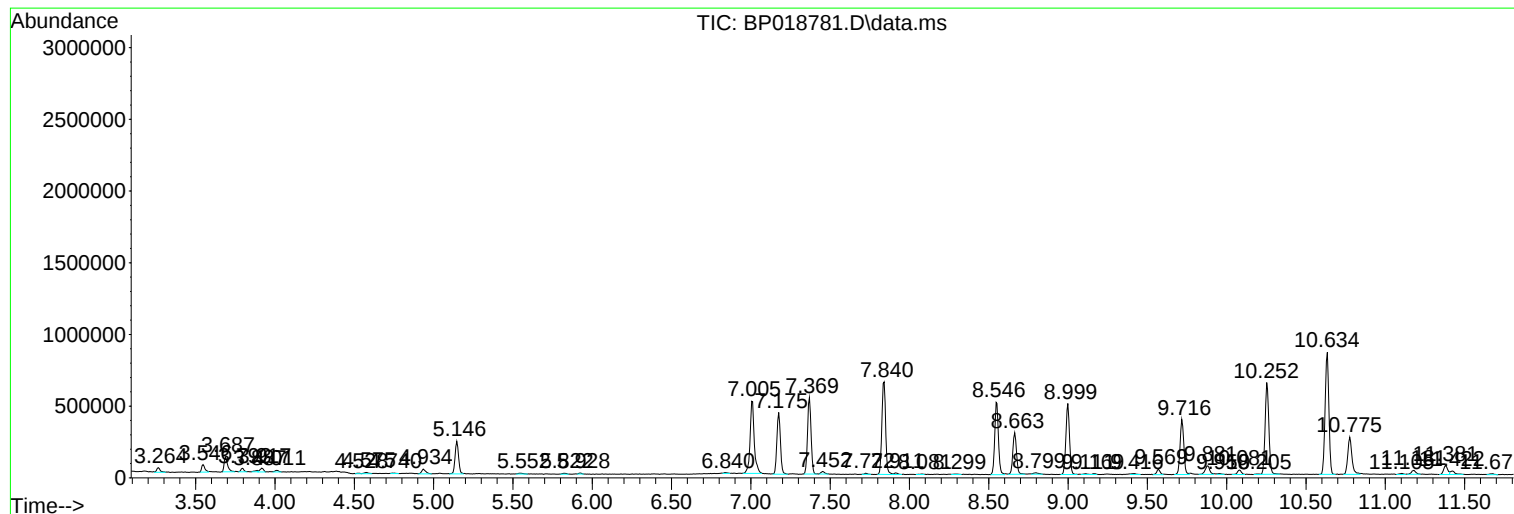
Sum of corrected areas: 44963877

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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



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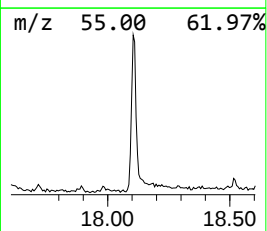
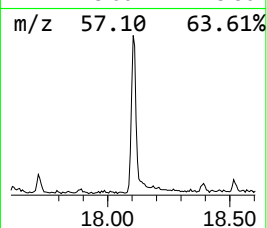
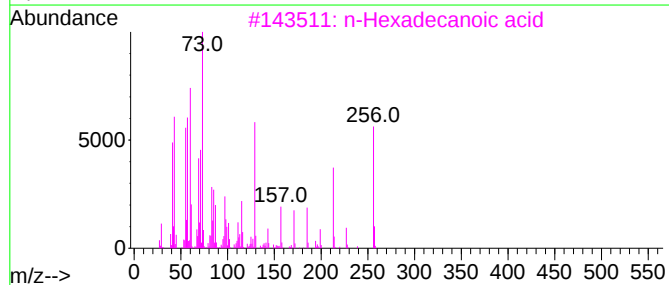
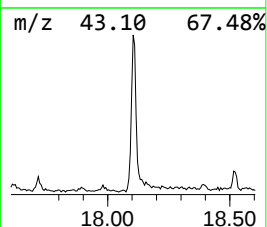
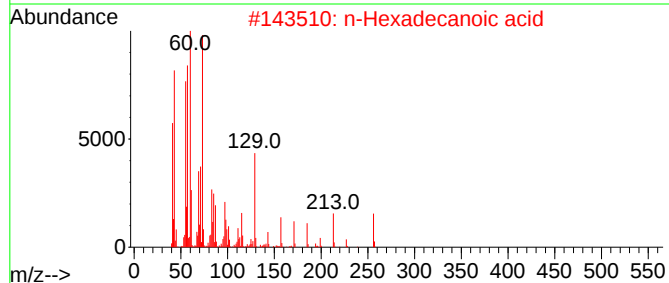
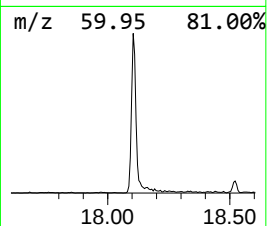
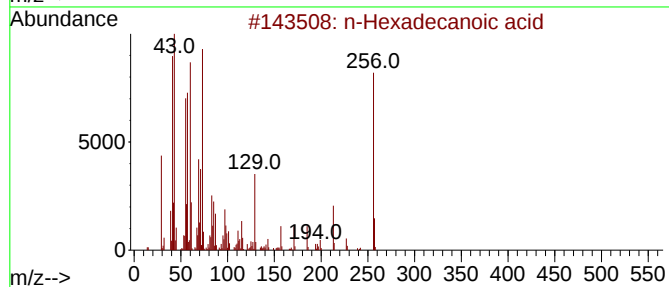
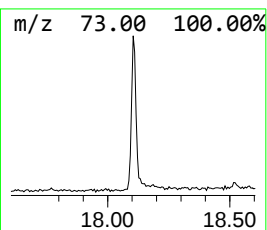
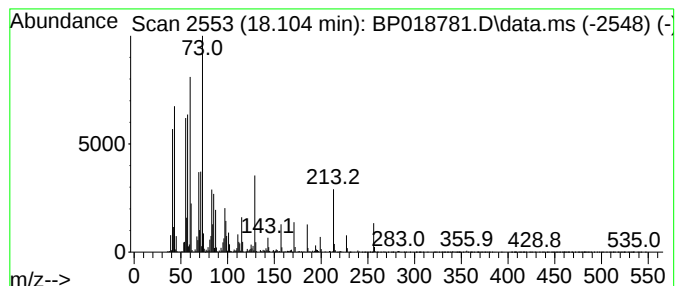
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	3.53 ng/ul	440288	Phenanthrene-d10	17.216

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



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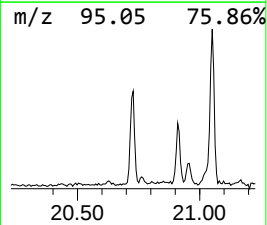
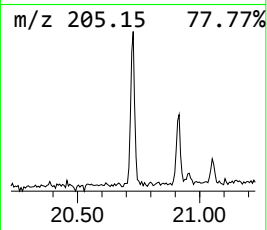
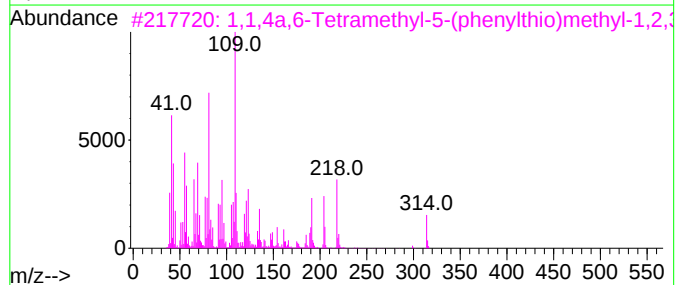
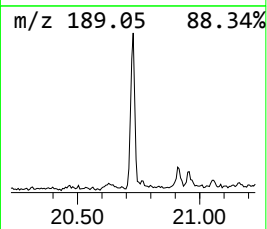
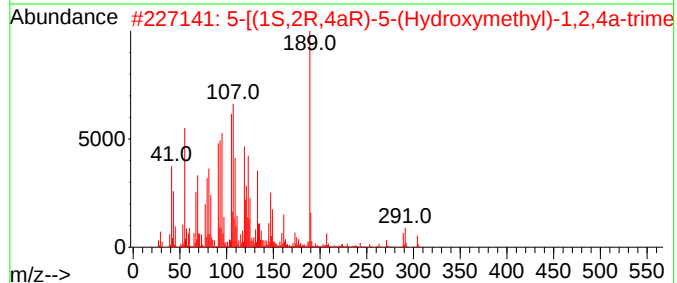
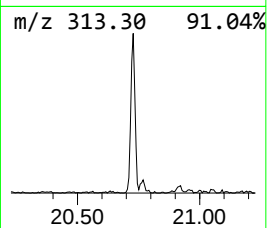
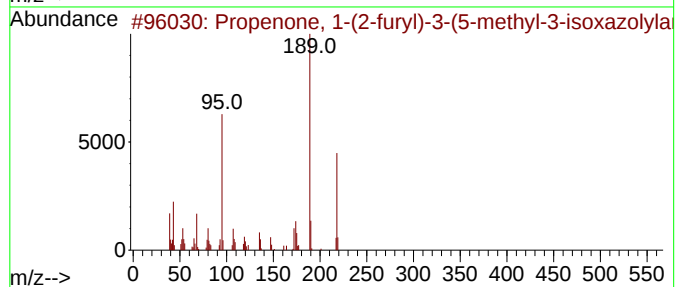
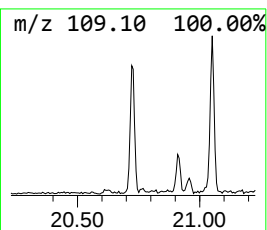
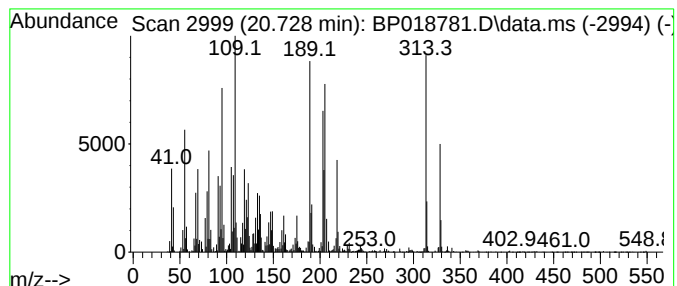
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.727	2.48 ng/ul	405230	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propenone, 1-(2-furyl)-3-(5-meth...	218	C11H10N2O3	186957-33-5	22
2			5-[(1S,2R,4aR)-5-(Hydroxymethyl)...	322	C20H34O3	132500-62-0	20
3			1,1,4a,6-Tetramethyl-5-(phenylth...	314	C21H30S	155191-62-1	18
4			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	15
5			2-Thiophenecarboxaldehyde, 4-bro...	218	C7H7BrOS	1000319-43-8	11



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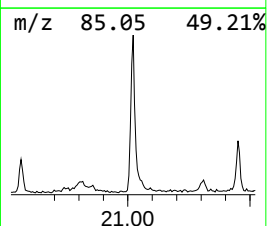
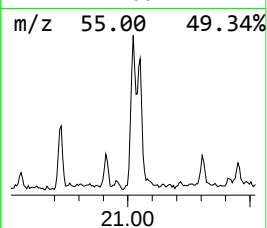
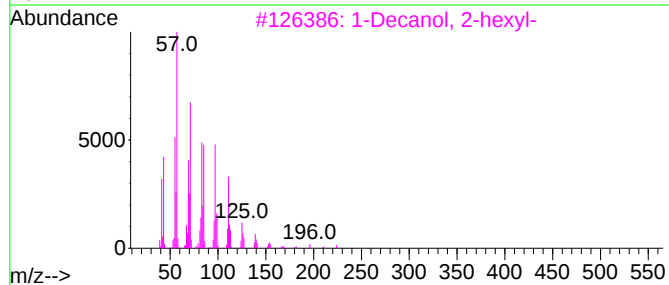
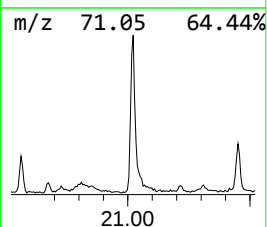
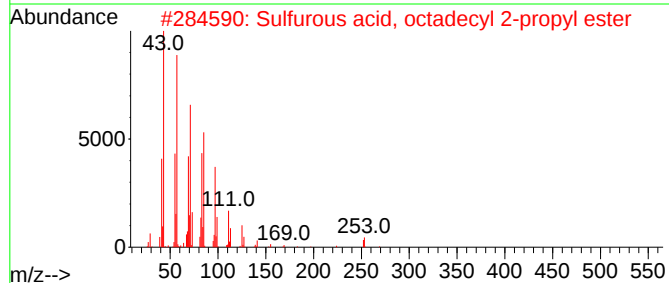
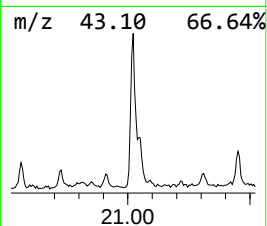
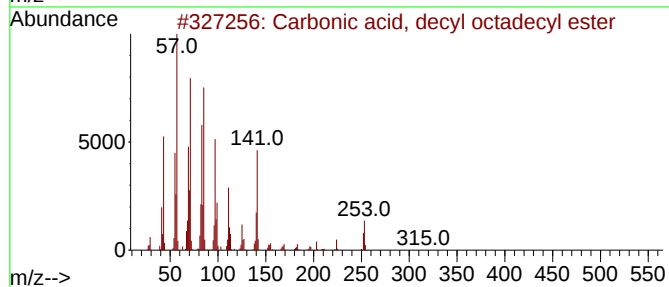
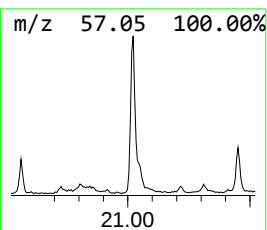
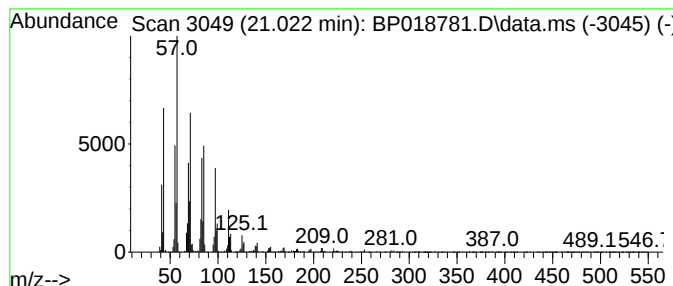
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 Carbonic acid, decyl octade... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.022	2.77 ng/ul	451898	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, decyl octadecyl e...	454	C29H58O3	1000383-16-7	91
2			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	91
3			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
4			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87
5			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018781.D
Acq On : 12 Dec 2023 23:06
Operator : MA/JU
Sample : 05646-04
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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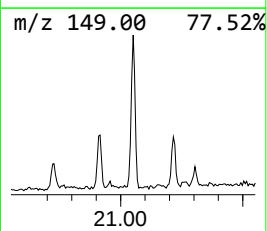
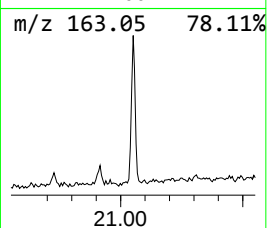
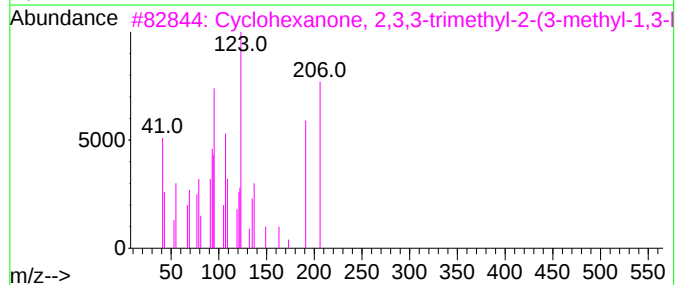
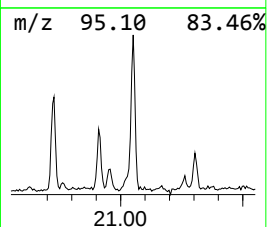
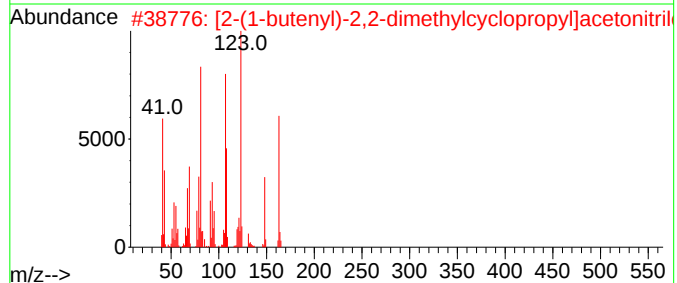
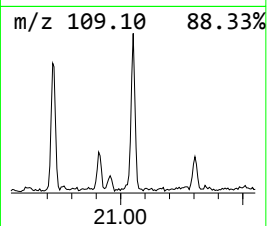
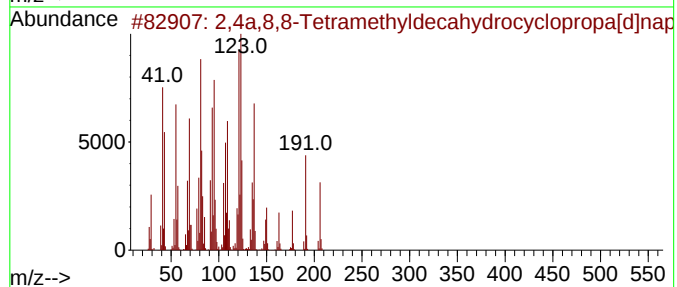
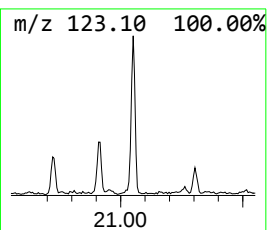
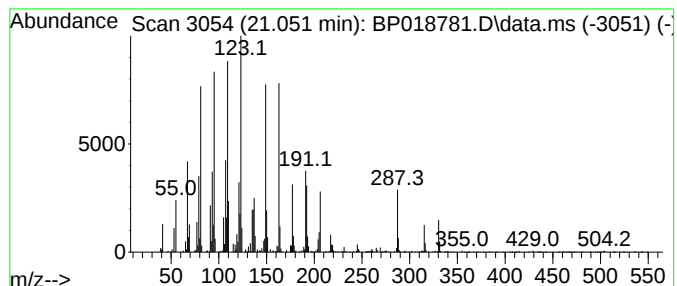
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	3.08 ng/ul	502936	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	43
2			[2-(1-butenyl)-2,2-dimethylcyclo...	163	C11H17N	1000111-15-4	30
3			Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-91-9	30
4			2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	27
5			Dispiro[2.2.5.0]undecan-4-one, 5...	220	C15H24O	1000152-13-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018781.D
Acq On : 12 Dec 2023 23:06
Operator : MA/JU
Sample : 05646-04
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AT8

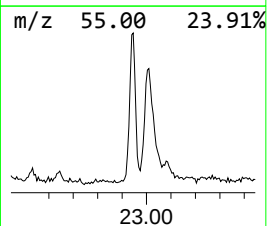
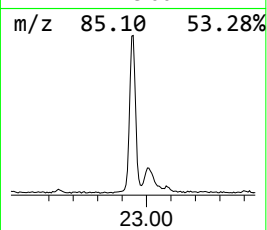
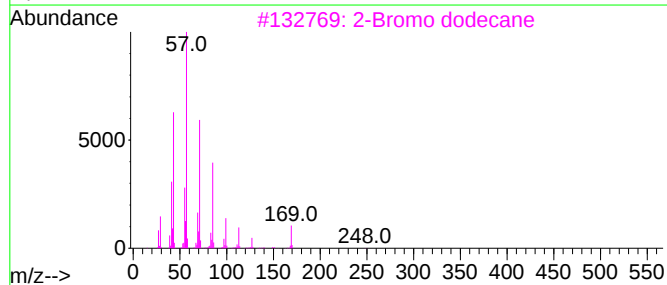
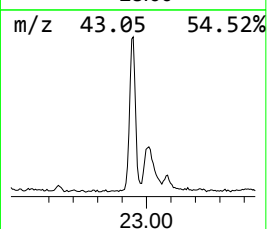
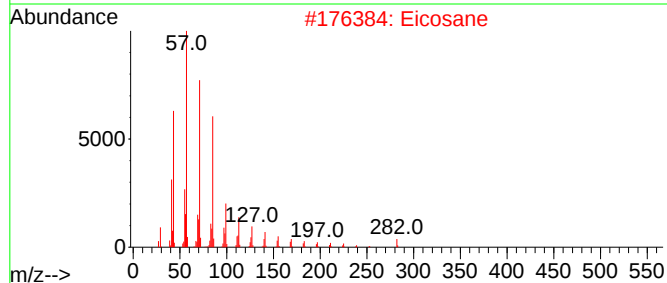
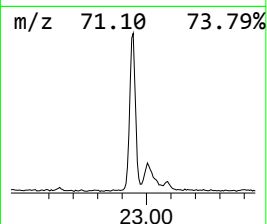
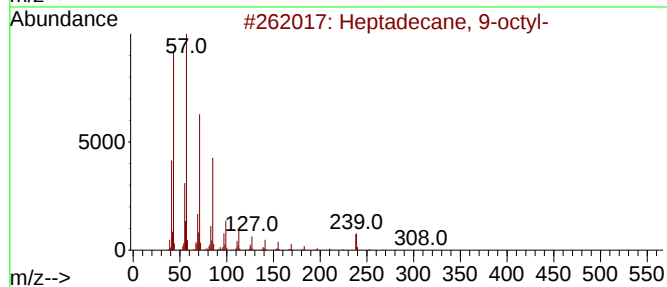
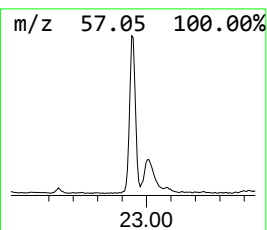
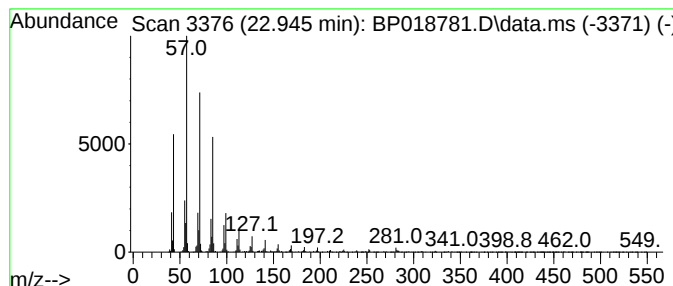
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Quant Title : SVOA CALIBRATION

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.
22.945	3.79 ng/ul	663944	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2			Eicosane	282	C20H42	000112-95-8	94
3			2-Bromo dodecane	248	C12H25Br	013187-99-0	93
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	93
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018781.D
Acq On : 12 Dec 2023 23:06
Operator : MA/JU
Sample : 05646-04
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AT8

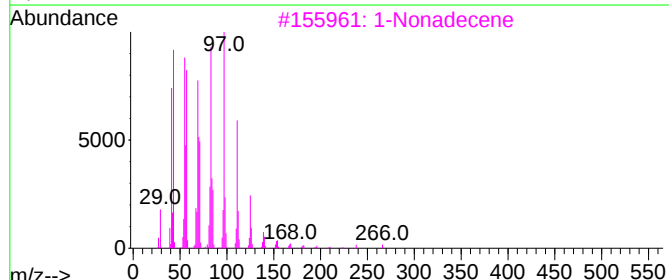
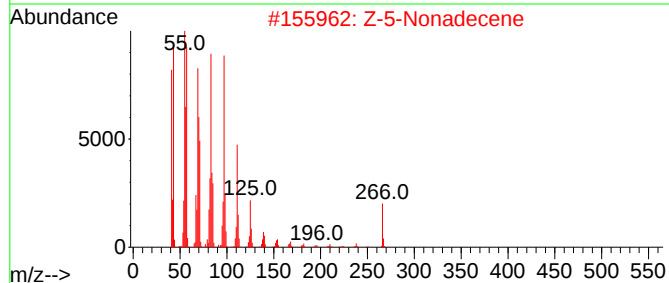
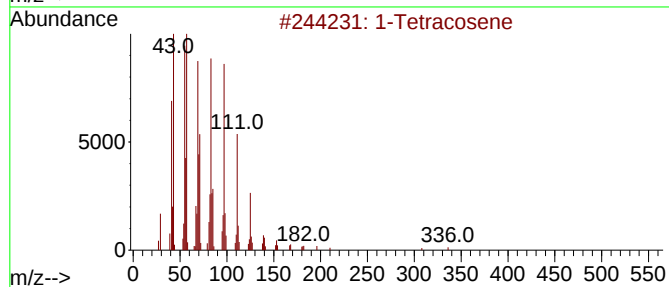
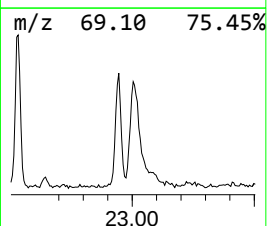
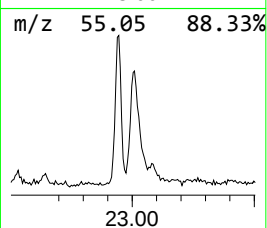
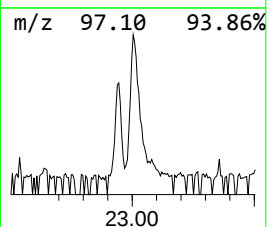
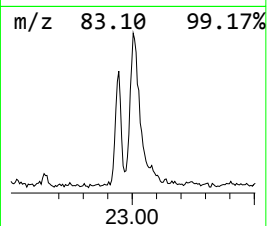
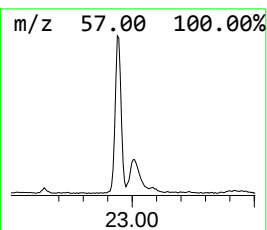
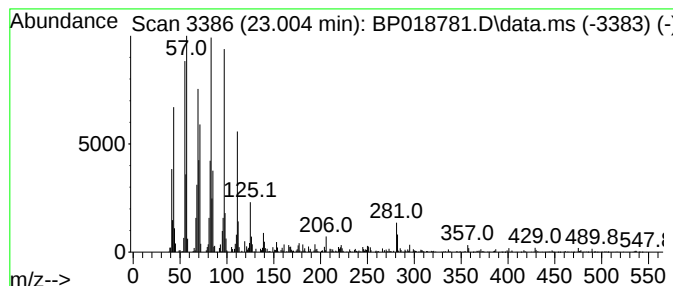
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.004	2.29 ng/ul	400551	Perylene-d12	23.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Tetracosene	336	C24H48	010192-32-2	99
2		Z-5-Nonadecene	266	C19H38	1000131-11-8	96
3		1-Nonadecene	266	C19H38	018435-45-5	95
4		1-Tetracosene	336	C24H48	010192-32-2	94
5		1-Hexacosene	364	C26H52	018835-33-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018781.D
Acq On : 12 Dec 2023 23:06
Operator : MA/JU
Sample : 05646-04
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AT8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.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 ...	18.104	3.5	ng/ul	440288	4	17.216	2492230	20.0
unknown-01	20.727	2.5	ng/ul	405230	5	21.298	3268470	20.0
Carbonic acid, ...	21.022	2.8	ng/ul	451898	5	21.298	3268470	20.0
unknown-02	21.051	3.1	ng/ul	502936	5	21.298	3268470	20.0
(DEL) Alkane: S...	22.945	3.8	ng/ul	663944	6	23.663	3501720	20.0
(DEL) Alkane: S...	23.004	2.3	ng/ul	400551	6	23.663	3501720	20.0