

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
 Data File : BM047108.D
 Acq On : 09 Aug 2024 06:11
 Operator : RC/JU
 Sample : P3435-09
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 E05X5

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_M\Methods\SFAM-EPA-BM080224.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM047108.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.016	18	22	28	rVB	41119	46016	1.23%	0.092%
2	3.281	65	67	75	rBV	28183	44762	1.19%	0.089%
3	3.405	84	88	103	rBV	481120	680807	18.17%	1.355%
4	3.699	135	138	150	rVB	23805	38181	1.02%	0.076%
5	4.022	189	193	196	rBV6	3947	5511	0.15%	0.011%
6	6.593	624	630	642	rVB	650303	984630	26.27%	1.960%
7	6.745	650	656	666	rVB	484964	744853	19.88%	1.483%
8	6.928	680	687	698	rBV	657750	1005673	26.84%	2.002%
9	7.034	700	705	710	rBV2	10826	17458	0.47%	0.035%
10	7.387	757	765	772	rBV	1030165	1600612	42.71%	3.186%
11	7.845	839	843	846	rBV6	4698	7283	0.19%	0.014%
12	8.104	880	887	898	rBV	786126	1242852	33.17%	2.474%
13	8.198	901	903	907	rVB5	7653	10089	0.27%	0.020%
14	8.528	950	959	970	rVV	593006	943957	25.19%	1.879%
15	9.116	1052	1059	1067	rBV9	8906	21675	0.58%	0.043%
16	9.239	1073	1080	1091	rBV	470612	762596	20.35%	1.518%
17	9.510	1124	1126	1134	rBV8	4987	6793	0.18%	0.014%
18	9.781	1164	1172	1184	rBV	767920	1288642	34.39%	2.565%
19	9.963	1199	1203	1207	rVB7	3694	5922	0.16%	0.012%
20	10.139	1225	1233	1241	rBV	1363681	2234274	59.62%	4.447%
21	10.292	1252	1259	1271	rBV	734755	1250099	33.36%	2.488%
22	10.722	1326	1332	1338	rBV9	9109	18297	0.49%	0.036%
23	10.904	1356	1363	1370	rBV	67864	133339	3.56%	0.265%
24	10.980	1370	1376	1382	rVB10	7030	17231	0.46%	0.034%
25	11.680	1490	1495	1499	rVB6	5339	8370	0.22%	0.017%
26	11.745	1499	1506	1511	rBV3	16550	29220	0.78%	0.058%
27	11.816	1515	1518	1521	rBV5	6386	7464	0.20%	0.015%
28	12.045	1550	1557	1561	rVB7	9192	15216	0.41%	0.030%
29	12.198	1575	1583	1588	rBV9	9596	20881	0.56%	0.042%
30	12.386	1609	1615	1619	rBV7	5988	12133	0.32%	0.024%
31	12.463	1624	1628	1632	rBV7	4308	6101	0.16%	0.012%
32	12.545	1636	1642	1646	rVV8	7903	12781	0.34%	0.025%
33	12.639	1656	1658	1659	rBV2	7774	6500	0.17%	0.013%
34	12.722	1669	1672	1676	rBV6	3380	5604	0.15%	0.011%
35	12.816	1684	1688	1689	rBV3	5079	4959	0.13%	0.010%
36	12.869	1692	1697	1699	rBV3	7523	12876	0.34%	0.026%

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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
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37	12.892	1699	1701	1707	rVB6	8464	11958	0.32%	0.024%
38	13.369	1780	1782	1789	rVB6	4573	8245	0.22%	0.016%
39	13.469	1792	1799	1812	rBV	1359502	1775377	47.38%	3.534%
40	13.727	1836	1843	1853	rBV	1539238	2257486	60.24%	4.494%
41	13.927	1872	1877	1878	rVB5	4630	6102	0.16%	0.012%
42	13.974	1878	1885	1888	rVV8	6477	10226	0.27%	0.020%
43	14.039	1888	1896	1903	rVV	2059706	2967993	79.20%	5.908%
44	14.104	1903	1907	1913	rVB5	12321	23048	0.62%	0.046%
45	14.286	1931	1938	1951	rBV2	419108	787303	21.01%	1.567%
46	14.445	1961	1965	1971	rVB4	9261	15488	0.41%	0.031%
47	14.504	1971	1975	1980	rBV8	10967	14216	0.38%	0.028%
48	14.574	1983	1987	1989	rBV4	4212	5554	0.15%	0.011%
49	14.816	2025	2028	2034	rVB8	5272	7223	0.19%	0.014%
50	14.880	2034	2039	2040	rVV4	9904	12522	0.33%	0.025%
51	14.898	2040	2042	2047	rVV2	11913	14641	0.39%	0.029%
52	14.933	2047	2048	2054	rVB5	5291	6859	0.18%	0.014%
53	15.045	2060	2067	2074	rBV	1945849	2727957	72.80%	5.430%
54	15.098	2074	2076	2081	rVB4	19348	25649	0.68%	0.051%
55	15.186	2085	2091	2099	rVV	260171	362856	9.68%	0.722%
56	15.286	2104	2108	2111	rVV4	10674	13247	0.35%	0.026%
57	15.327	2111	2115	2118	rVB4	5970	7779	0.21%	0.015%
58	15.615	2160	2164	2166	rBV4	8444	12766	0.34%	0.025%
59	15.739	2180	2185	2187	rBV6	3513	6421	0.17%	0.013%
60	15.804	2192	2196	2199	rBV	27861	31856	0.85%	0.063%
61	15.957	2219	2222	2223	rBV2	5581	5826	0.16%	0.012%
62	16.004	2227	2230	2231	rVV3	9371	8813	0.24%	0.018%
63	16.027	2232	2234	2239	rVV6	8007	9852	0.26%	0.020%
64	16.110	2242	2248	2252	rVB9	9259	13233	0.35%	0.026%
65	16.157	2253	2256	2260	rVB5	6376	7699	0.21%	0.015%
66	16.239	2268	2270	2276	rBV5	14820	20693	0.55%	0.041%
67	16.310	2278	2282	2284	rBV5	4016	6561	0.18%	0.013%
68	16.351	2286	2289	2292	rVB5	4158	5146	0.14%	0.010%
69	16.468	2304	2309	2310	rBV4	23896	33796	0.90%	0.067%
70	16.486	2310	2312	2316	rVV4	28937	30928	0.83%	0.062%
71	16.551	2320	2323	2325	rBV4	5572	5000	0.13%	0.010%
72	16.598	2325	2331	2337	rVB7	14531	28984	0.77%	0.058%
73	16.798	2359	2365	2371	rBV	2359683	3501371	93.43%	6.970%
74	16.898	2376	2382	2392	rVV	2154308	3062635	81.73%	6.096%
75	17.015	2399	2402	2406	rVB6	10162	12137	0.32%	0.024%
76	17.062	2406	2410	2416	rBV4	33183	42353	1.13%	0.084%

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77	17.204	2428	2434	2441	rBV4	73768	106854	2.85%	0.213%
78	17.339	2454	2457	2459	rBV4	11451	12383	0.33%	0.025%
79	17.615	2498	2504	2509	rBV4	41010	80037	2.14%	0.159%
80	17.674	2511	2514	2519	rVB7	21741	33047	0.88%	0.066%
81	17.739	2519	2525	2532	rBV	328695	505275	13.48%	1.006%
82	17.798	2533	2535	2541	rVB2	32143	49275	1.31%	0.098%
83	18.656	2677	2681	2682	rBV4	39905	44011	1.17%	0.088%
84	18.680	2682	2685	2692	rVB	88259	111405	2.97%	0.222%
85	18.774	2696	2701	2708	rVB5	40873	66542	1.78%	0.132%
86	18.845	2710	2713	2714	rBV	26039	30172	0.81%	0.060%
87	18.874	2714	2718	2723	rVB	302886	380758	10.16%	0.758%
88	19.033	2741	2745	2755	rBV	186496	334888	8.94%	0.667%
89	19.209	2769	2775	2789	rBV2	2453393	3663142	97.75%	7.292%
90	19.498	2821	2824	2828	rVB4	41543	46359	1.24%	0.092%
91	19.745	2864	2866	2870	rBV	37615	44698	1.19%	0.089%
92	19.809	2873	2877	2881	rVB	206279	211798	5.65%	0.422%
93	20.774	3037	3041	3050	rVB	356061	460494	12.29%	0.917%
94	21.033	3079	3085	3089	rBV	2612399	3747439	100.00%	7.460%
95	21.074	3089	3092	3101	rVB	217991	295706	7.89%	0.589%
96	21.768	3207	3210	3219	rVB2	216121	415322	11.08%	0.827%
97	22.156	3271	3276	3283	rVB	811039	1217739	32.50%	2.424%
98	23.015	3417	3422	3428	rBV	456971	759624	20.27%	1.512%
99	23.550	3506	3513	3520	rBV	1393083	2919999	77.92%	5.812%
100	23.733	3537	3544	3553	rBV	1552556	3538409	94.42%	7.043%

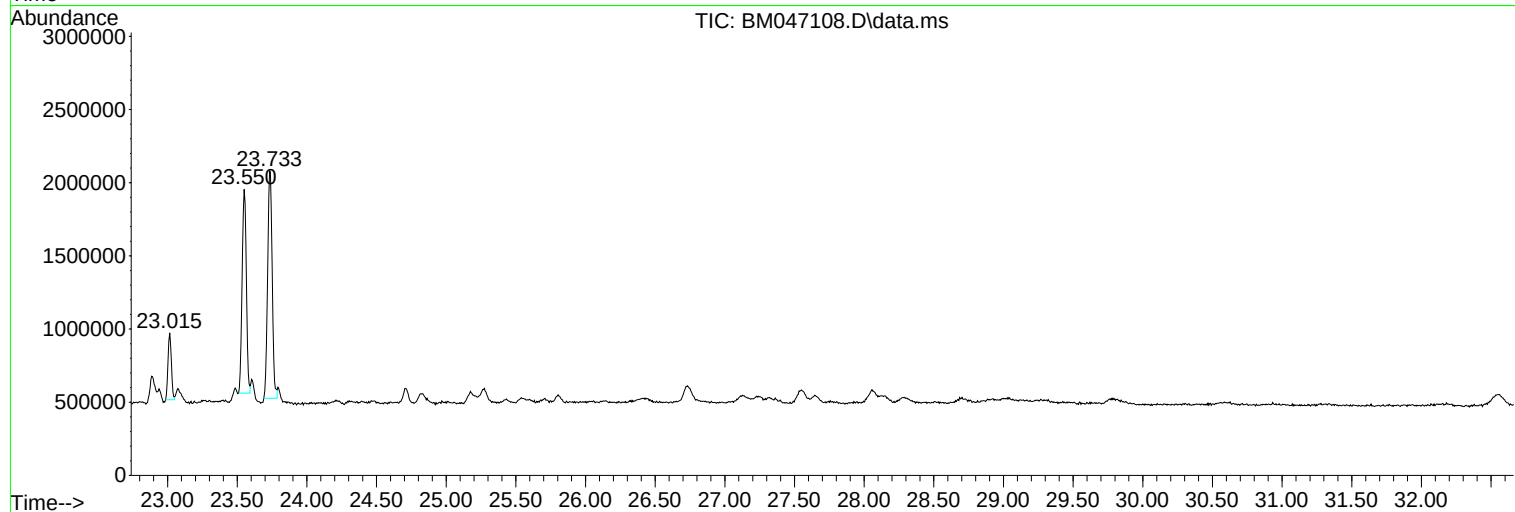
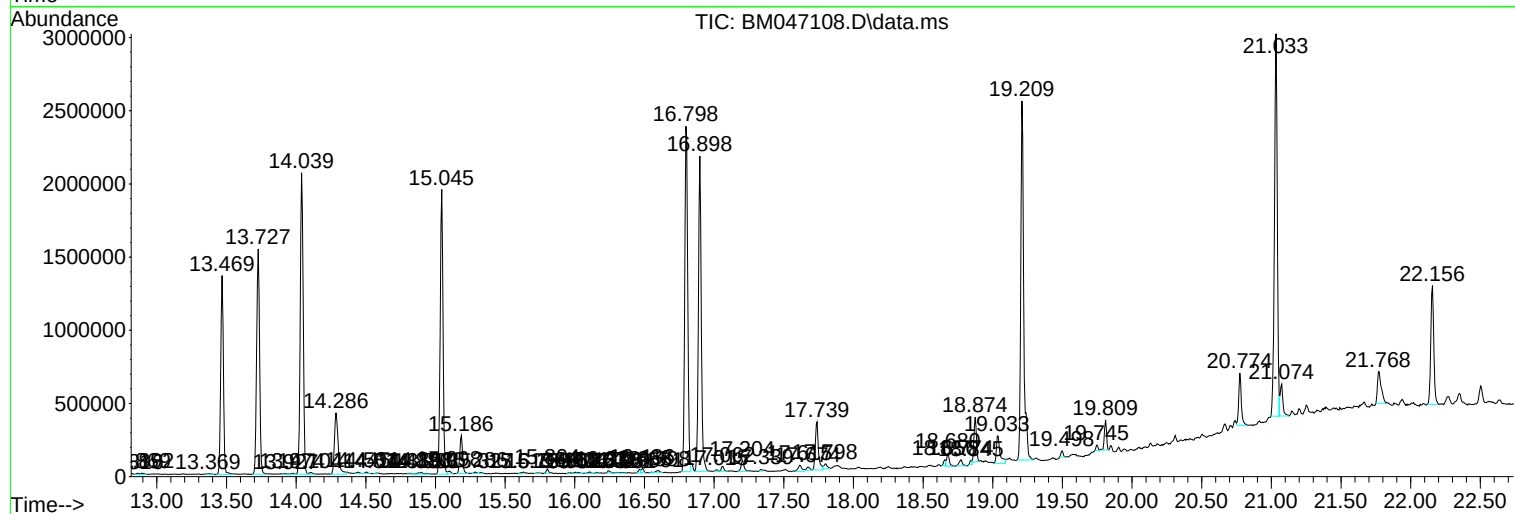
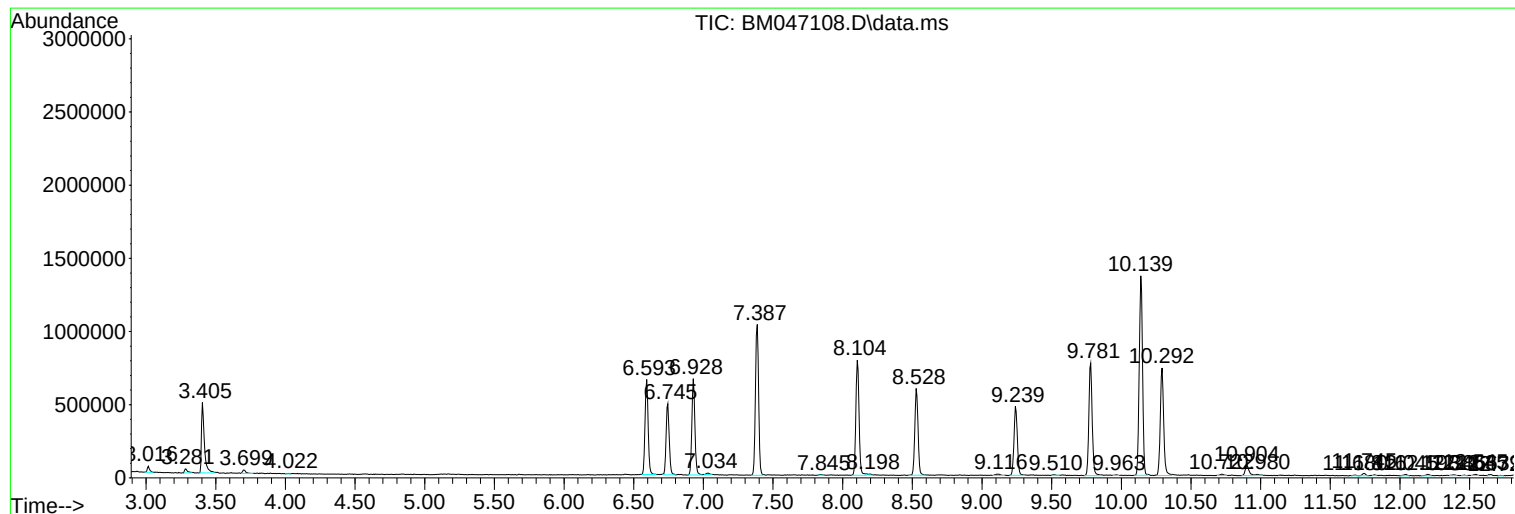
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
Quant Title : SVOA CALIBRATION

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



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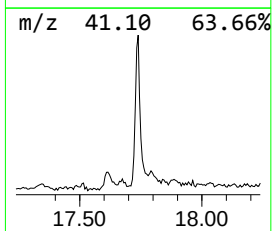
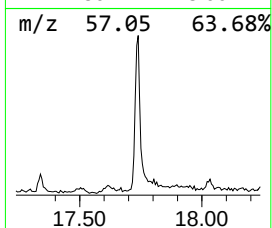
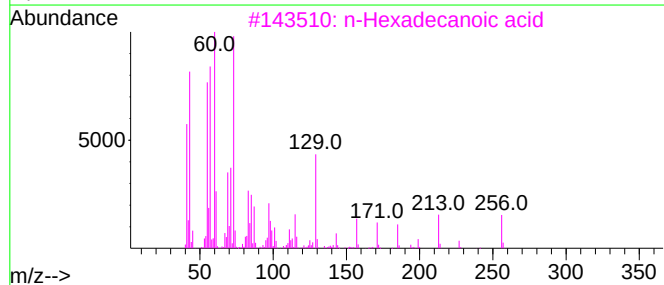
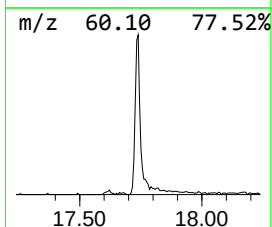
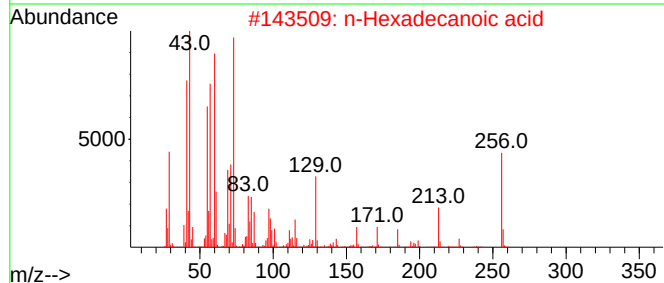
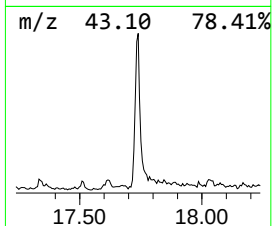
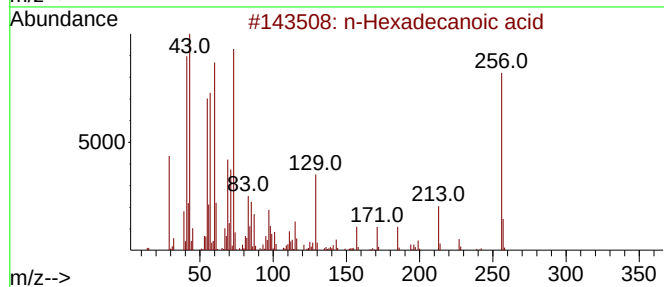
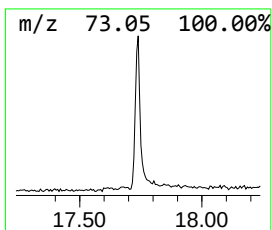
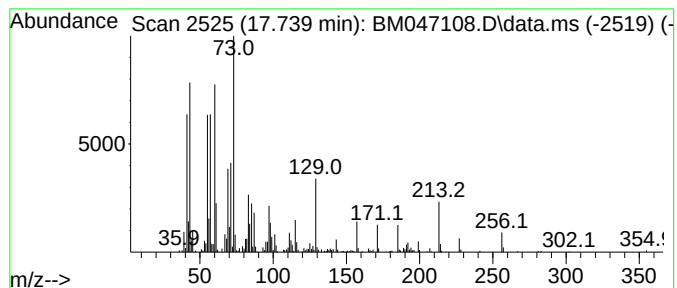
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.739	2.89 ng/ul	505275	Phenanthrene-d10	16.798	
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	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
5	Tridecanoic acid	214	C13H26O2	000638-53-9	94



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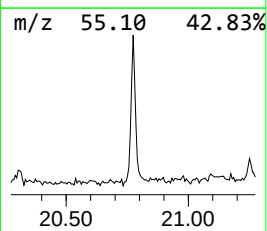
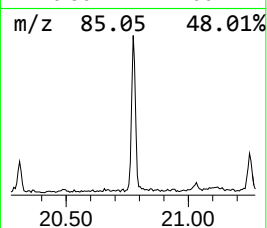
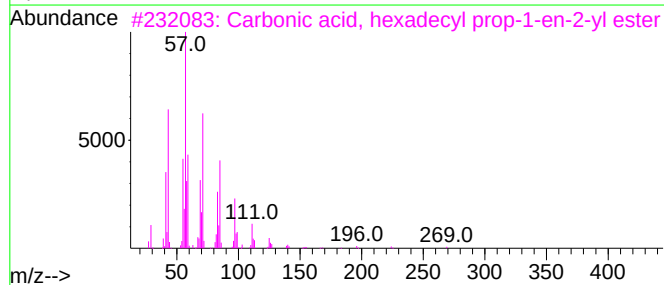
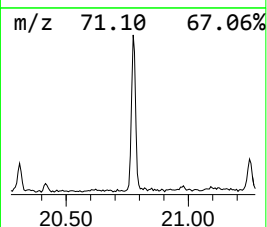
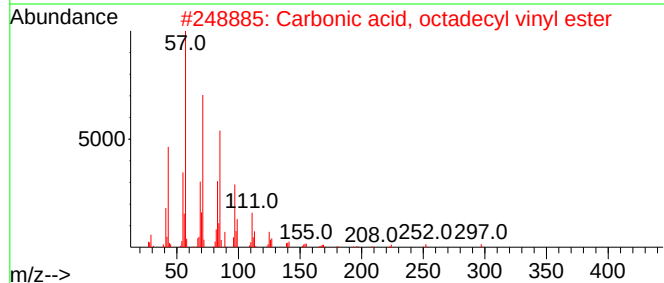
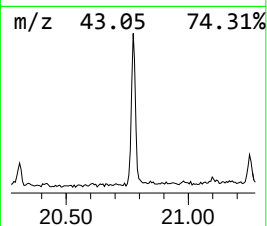
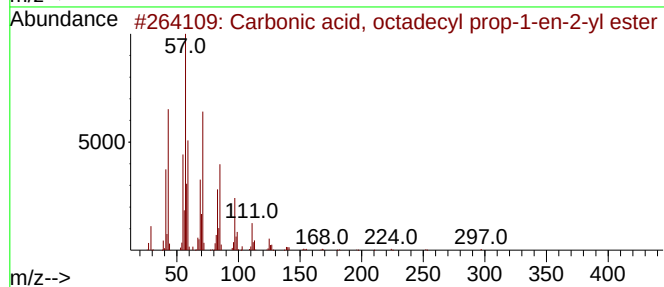
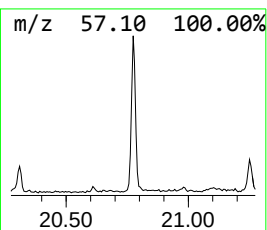
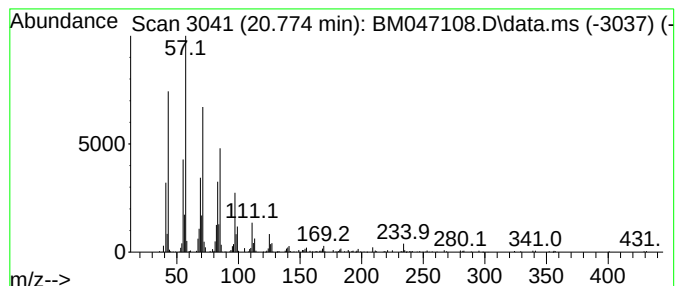
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Carbonic acid, octadecyl pr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.774	2.46 ng/ul	460494	Chrysene-d12	21.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	94
2			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	91
3			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	91
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	91



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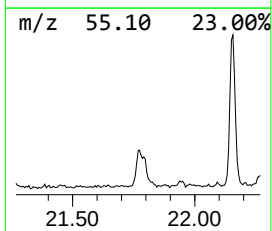
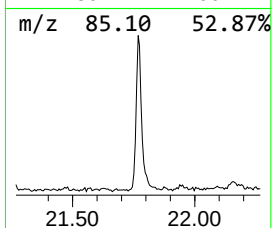
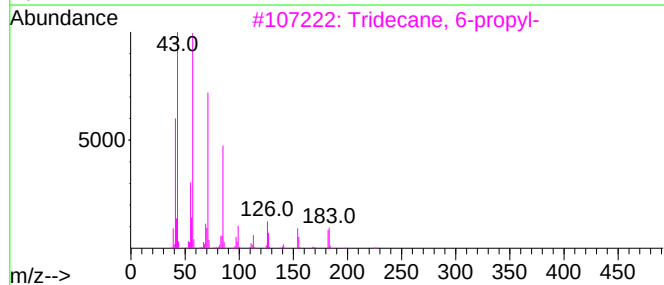
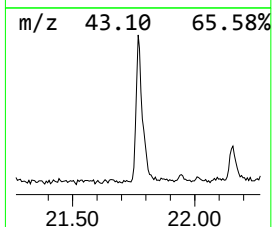
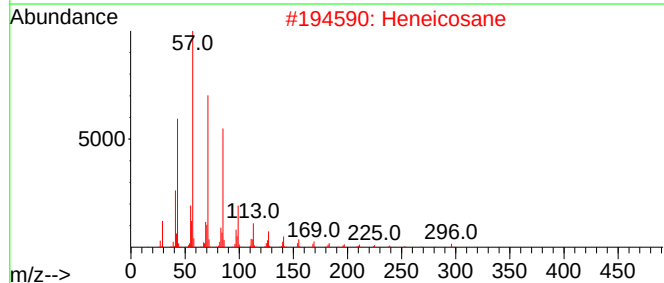
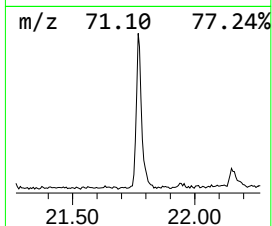
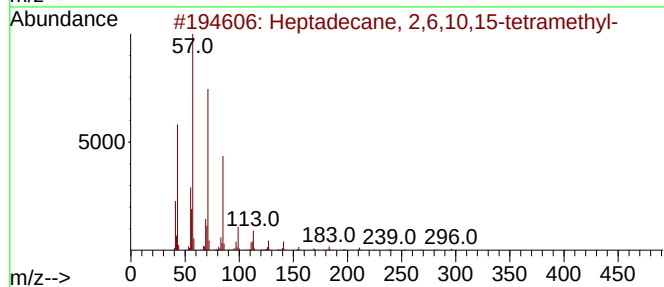
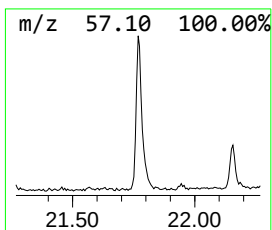
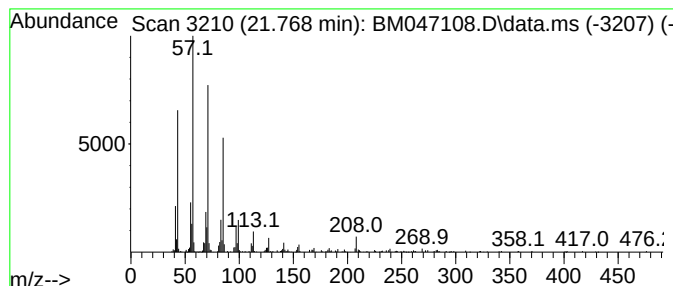
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.768	2.22 ng/ul	415322	Chrysene-d12	21.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
2			Heneicosane	296	C21H44	000629-94-7	90
3			Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
4			Hexatriacontane	507	C36H74	000630-06-8	87
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047108.D
Acq On : 09 Aug 2024 06:11
Operator : RC/JU
Sample : P3435-09
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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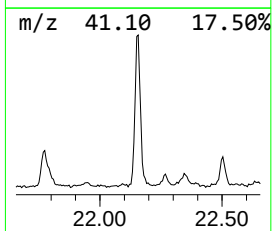
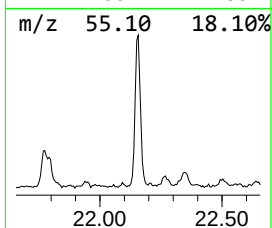
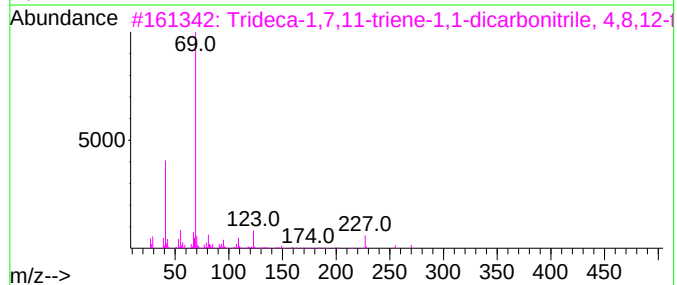
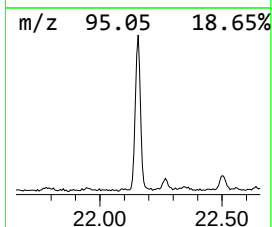
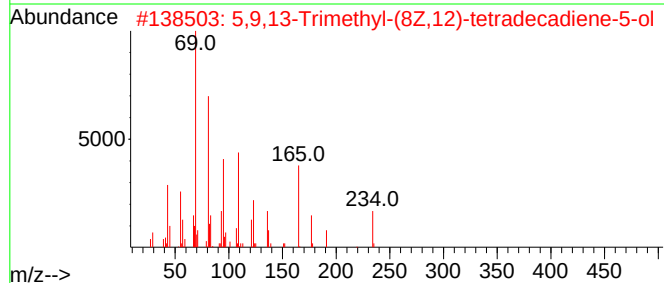
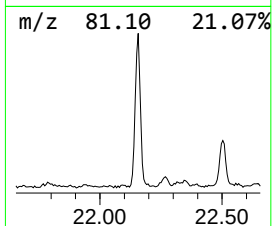
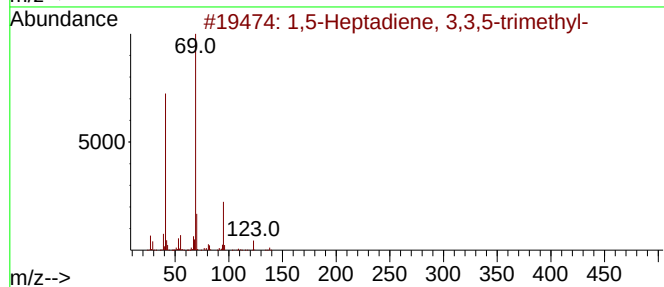
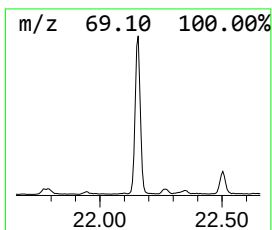
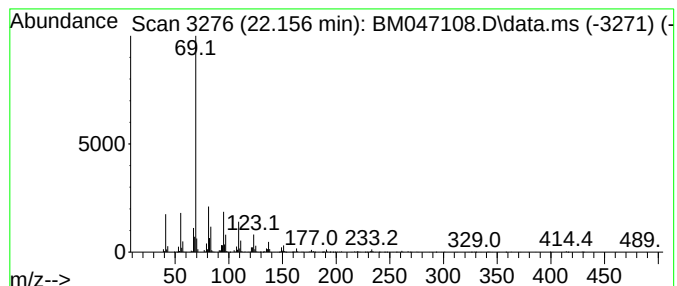
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 1,5-Heptadiene, 3,3,5-trime... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.156	6.50 ng/ul	1217740	Chrysene-d12	21.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	59		
2	5,9,13-Trimethyl-(8Z,12)-tetradec...	252	C17H32O	1000432-48-1	56		
3	Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	53		
4	3-Isopropyl-5-methyl-hex-4-en-2-one	154	C10H18O	077142-85-9	53		
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047108.D
Acq On : 09 Aug 2024 06:11
Operator : RC/JU
Sample : P3435-09
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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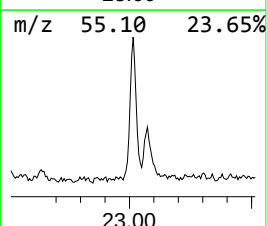
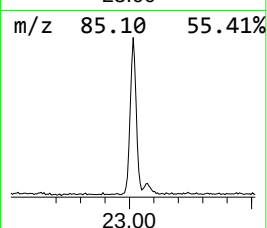
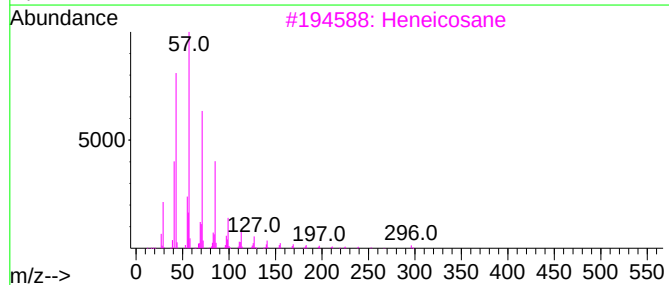
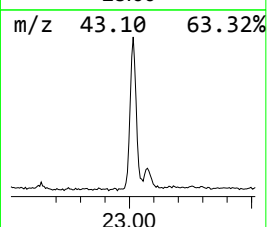
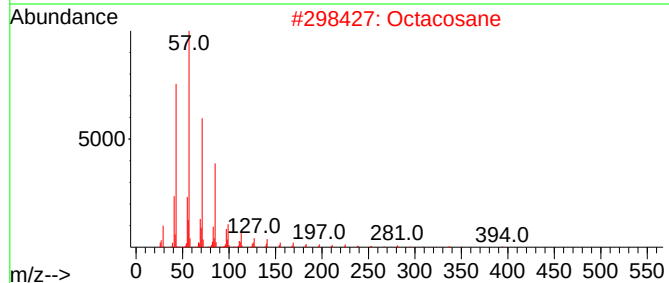
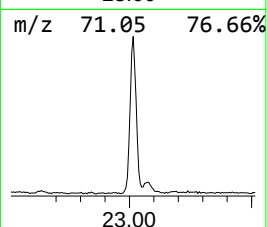
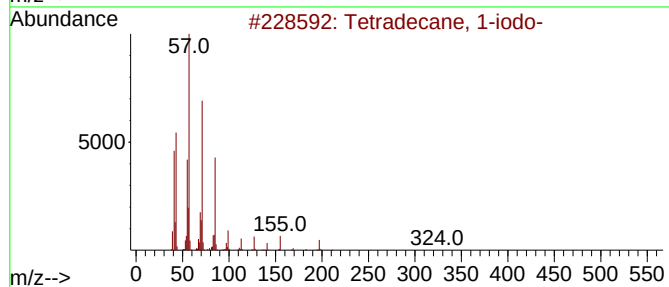
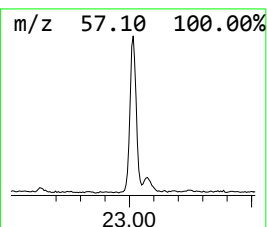
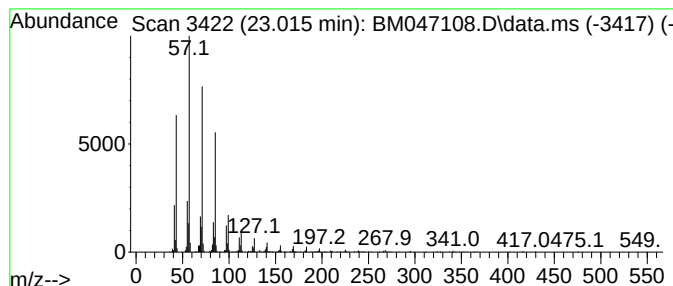
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Tetradecane, 1-iodo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.015	4.29 ng/ul	759624	Perylene-d12	23.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	93
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047108.D
Acq On : 09 Aug 2024 06:11
Operator : RC/JU
Sample : P3435-09
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E05X5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.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 ...	17.739	2.9	ng/ul	505275	4	16.798	3501370	20.0
Carbonic acid, ...	20.774	2.5	ng/ul	460494	5	21.033	3747440	20.0
(DEL) Alkane: S...	21.768	2.2	ng/ul	415322	5	21.033	3747440	20.0
1,5-Heptadiene,...	22.156	6.5	ng/ul	1217740	5	21.033	3747440	20.0
Tetradecane, 1-...	23.015	4.3	ng/ul	759624	6	23.733	3538410	20.0