

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
 Data File : BM038174.D
 Acq On : 21 Dec 2022 16:25
 Operator : CG/JU
 Sample : N6014-21
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DBXT3

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-BM120722.M
 Title : SVOA CALIBRATION

Signal : TIC: BM038174.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	32	36	52	rVB	41422	74982	1.34%	0.116%
2	3.828	105	109	135	rBV	562826	997902	17.87%	1.544%
3	4.157	162	165	173	rVB2	14528	25994	0.47%	0.040%
4	7.204	676	683	693	rBV	1094806	1703563	30.50%	2.635%
5	7.369	703	711	723	rVB	686986	1054466	18.88%	1.631%
6	7.569	738	745	757	rBV	1077688	1674025	29.98%	2.590%
7	8.040	818	825	834	rBV	804099	1233585	22.09%	1.908%
8	8.757	939	947	957	rBV	1392474	2179928	39.03%	3.372%
9	9.216	1017	1025	1032	rBV	1025045	1634836	29.27%	2.529%
10	9.369	1047	1051	1060	rVB9	9069	15291	0.27%	0.024%
11	9.587	1085	1088	1096	rVB9	4596	10801	0.19%	0.017%
12	9.939	1139	1148	1157	rBV	900619	1467665	26.28%	2.270%
13	10.475	1232	1239	1248	rBV	1509394	2538706	45.46%	3.927%
14	10.857	1296	1304	1312	rBV	1128809	1796503	32.17%	2.779%
15	10.939	1314	1318	1321	rBV5	10221	13663	0.24%	0.021%
16	10.998	1321	1328	1342	rBV	1131665	1920261	34.38%	2.970%
17	11.633	1431	1436	1440	rBV7	4764	8136	0.15%	0.013%
18	12.086	1506	1513	1516	rBV9	2801	6262	0.11%	0.010%
19	12.433	1567	1572	1576	rBV2	27742	41907	0.75%	0.065%
20	12.945	1656	1659	1664	rBV5	5773	7893	0.14%	0.012%
21	13.480	1744	1750	1753	rVB4	4451	7808	0.14%	0.012%
22	13.633	1772	1776	1784	rVB7	5746	15377	0.28%	0.024%
23	13.986	1831	1836	1842	rBV8	11747	19947	0.36%	0.031%
24	14.080	1843	1852	1861	rVV	2626889	3403492	60.94%	5.265%
25	14.186	1865	1870	1876	rVB10	6745	13442	0.24%	0.021%
26	14.304	1887	1890	1894	rBV7	7591	11078	0.20%	0.017%
27	14.369	1894	1901	1911	rVB	3044230	4265921	76.39%	6.599%
28	14.539	1925	1930	1935	rVB7	8698	18198	0.33%	0.028%
29	14.669	1944	1952	1960	rBV	1613508	2297439	41.14%	3.554%
30	14.874	1978	1987	2003	rBV	991030	1510599	27.05%	2.337%
31	15.027	2007	2013	2017	rVV4	13138	22442	0.40%	0.035%
32	15.069	2017	2020	2026	rVB7	18736	26851	0.48%	0.042%
33	15.233	2044	2048	2051	rBV6	3329	6190	0.11%	0.010%
34	15.298	2054	2059	2062	rVV6	7507	12970	0.23%	0.020%
35	15.333	2062	2065	2070	rVB6	7144	9858	0.18%	0.015%
36	15.433	2077	2082	2083	rBV5	3974	5589	0.10%	0.009%

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37	15.492	2088	2092	2095	rVB4	7113	10755	0.19%	0.017%
38	15.657	2114	2120	2128	rBV	3581071	5097362	91.27%	7.885%
39	15.780	2134	2141	2147	rBV	603000	826121	14.79%	1.278%
40	15.892	2154	2160	2166	rBV4	18452	30943	0.55%	0.048%
41	16.021	2176	2182	2188	rVB	87408	122989	2.20%	0.190%
42	16.192	2207	2211	2215	rBV7	5373	10113	0.18%	0.016%
43	16.280	2223	2226	2232	rVB8	8275	12242	0.22%	0.019%
44	16.351	2235	2238	2243	rBV5	11033	18072	0.32%	0.028%
45	16.445	2249	2254	2259	rVB9	5867	12102	0.22%	0.019%
46	16.498	2259	2263	2268	rBV8	15101	28801	0.52%	0.045%
47	16.580	2274	2277	2282	rVB6	10017	13871	0.25%	0.021%
48	16.668	2288	2292	2295	rVB5	7381	9962	0.18%	0.015%
49	16.792	2309	2313	2319	rBV2	50410	73606	1.32%	0.114%
50	17.086	2360	2363	2368	rVB7	7542	10096	0.18%	0.016%
51	17.145	2370	2373	2377	rBV5	7410	13330	0.24%	0.021%
52	17.257	2389	2392	2394	rBV3	7991	9079	0.16%	0.014%
53	17.286	2394	2397	2404	rVB3	39824	53255	0.95%	0.082%
54	17.351	2405	2408	2412	rBV2	26346	31621	0.57%	0.049%
55	17.410	2412	2418	2427	rBV	1796128	2533827	45.37%	3.920%
56	17.510	2427	2435	2442	rBV	3745507	5090062	91.14%	7.874%
57	17.598	2448	2450	2457	rVB7	15544	25205	0.45%	0.039%
58	17.668	2458	2462	2468	rBV6	14949	31703	0.57%	0.049%
59	17.751	2472	2476	2479	rBV6	23447	31276	0.56%	0.048%
60	17.880	2496	2498	2499	rBV2	5637	5722	0.10%	0.009%
61	17.915	2502	2504	2512	rVB6	17722	29088	0.52%	0.045%
62	18.004	2516	2519	2525	rVV4	15176	33852	0.61%	0.052%
63	18.057	2526	2528	2534	rVB6	16778	24352	0.44%	0.038%
64	18.162	2541	2546	2553	rBV3	73920	147567	2.64%	0.228%
65	18.227	2553	2557	2562	rBV	66574	93203	1.67%	0.144%
66	18.286	2562	2567	2577	rBV	789565	1095353	19.61%	1.694%
67	18.580	2613	2617	2622	rBV8	23694	43406	0.78%	0.067%
68	18.627	2623	2625	2631	rVV6	16605	28015	0.50%	0.043%
69	18.704	2634	2638	2644	rBV4	37601	48353	0.87%	0.075%
70	19.298	2736	2739	2742	rBV2	30450	34857	0.62%	0.054%
71	19.339	2742	2746	2747	rBV3	42017	52806	0.95%	0.082%
72	19.433	2755	2762	2763	rBV3	125377	221516	3.97%	0.343%
73	19.456	2763	2766	2772	rVB	180458	265769	4.76%	0.411%
74	19.551	2779	2782	2788	rBV	179065	237205	4.25%	0.367%
75	19.792	2817	2823	2835	rBV	4041551	5584688	100.00%	8.639%
76	20.280	2903	2906	2909	rBV3	63743	101017	1.81%	0.156%

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77	20.762	2985	2988	2991	rBV	170931	168559	3.02%	0.261%
78	21.262	3069	3073	3078	rBV	471813	653231	11.70%	1.010%
79	21.574	3121	3126	3131	rBV	1536032	2241733	40.14%	3.468%
80	22.174	3225	3228	3231	rBV2	126058	138848	2.49%	0.215%
81	22.821	3335	3338	3345	rVB	198777	265691	4.76%	0.411%
82	23.239	3405	3409	3412	rBV	305211	432075	7.74%	0.668%
83	23.874	3510	3517	3524	rBV2	2175707	4196604	75.14%	6.492%
84	24.033	3538	3544	3551	rVB2	965647	1916322	34.31%	2.964%
85	24.609	3639	3642	3653	rVB	345270	667710	11.96%	1.033%
86	27.121	4063	4069	4082	rVB2	585087	1766902	31.64%	2.733%

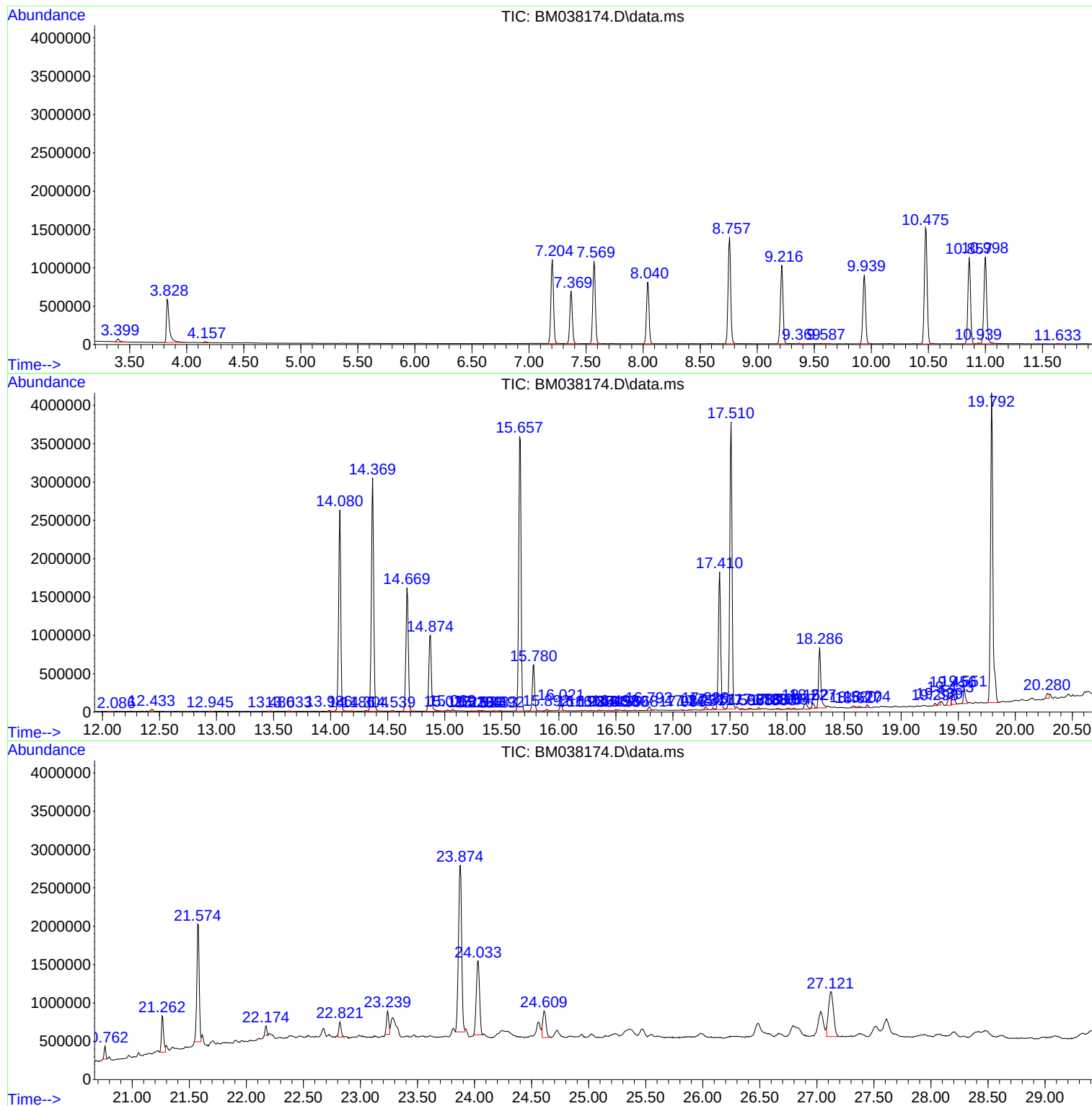
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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



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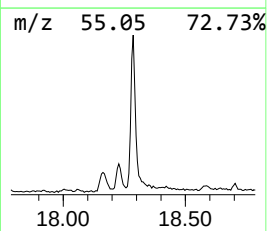
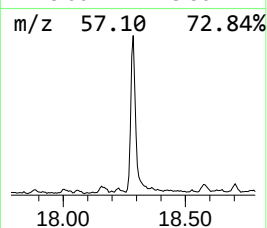
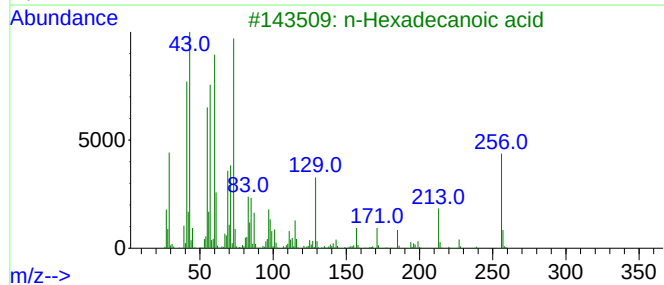
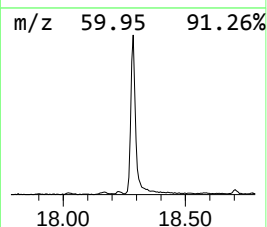
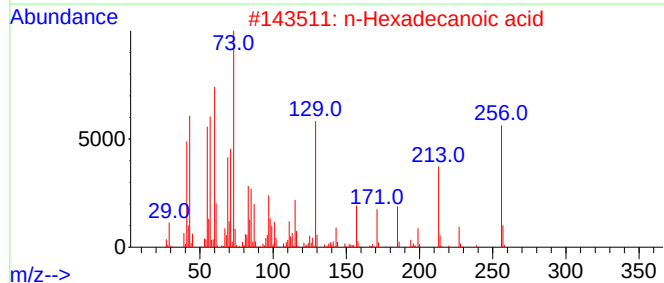
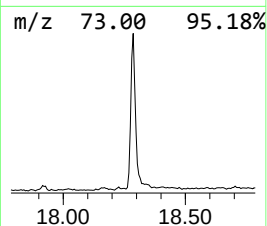
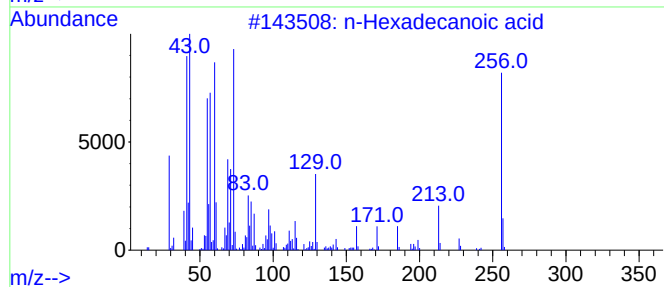
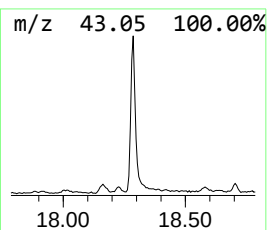
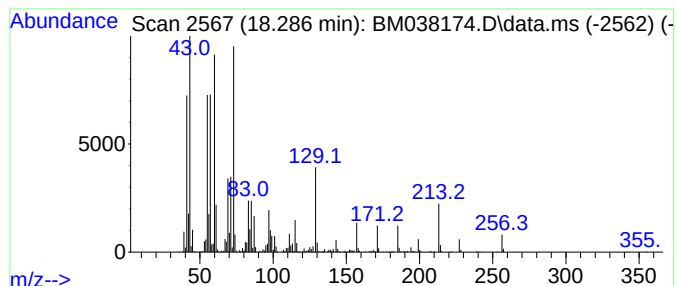
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	8.65 ng/ul	1095350	Phenanthrene-d10	17.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5		Octadecanoic acid	284	C18H36O2	000057-11-4	93



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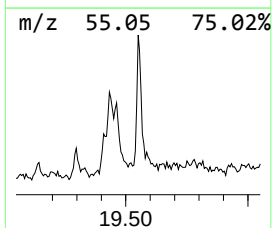
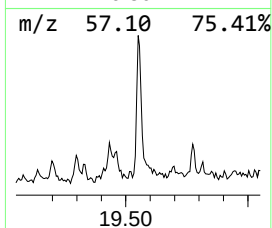
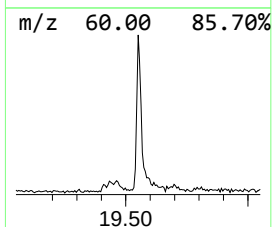
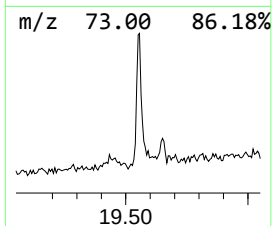
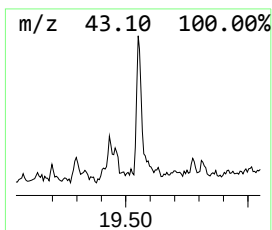
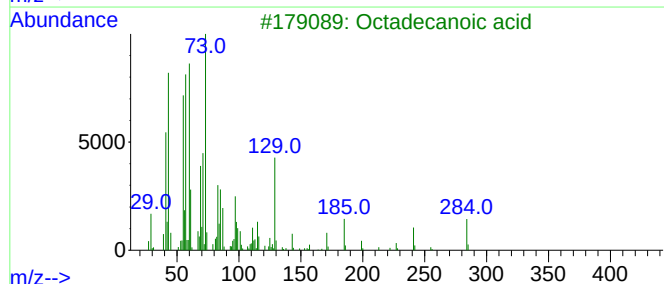
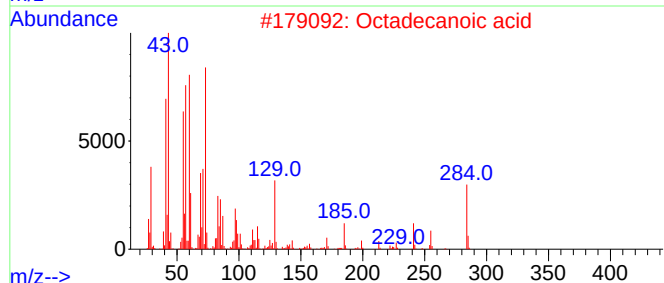
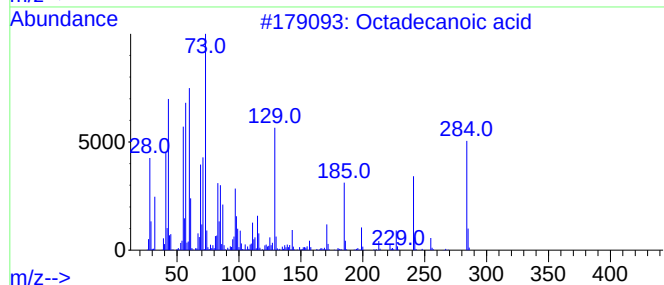
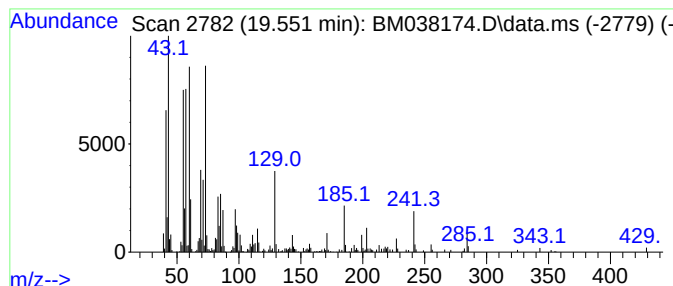
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	2.12 ng/ul	237205	Chrysene-d12	21.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	97
3			Octadecanoic acid	284	C18H36O2	000057-11-4	96
4			Octadecanoic acid	284	C18H36O2	000057-11-4	91
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87



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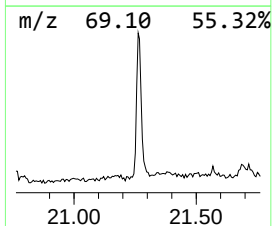
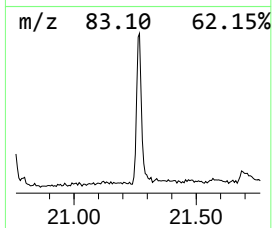
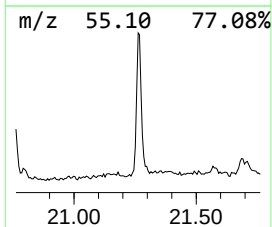
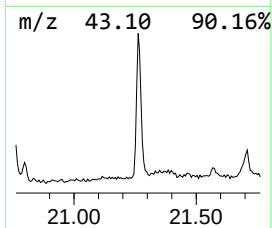
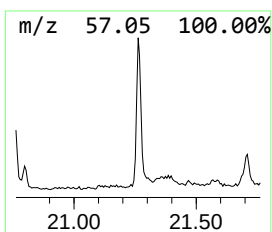
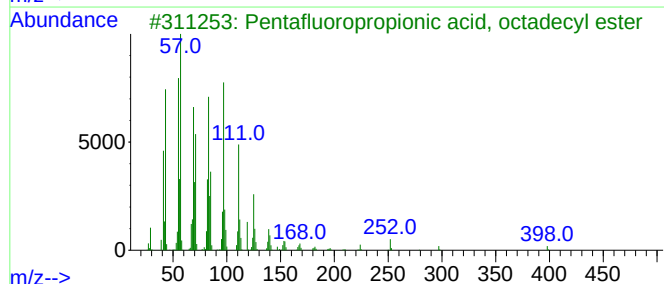
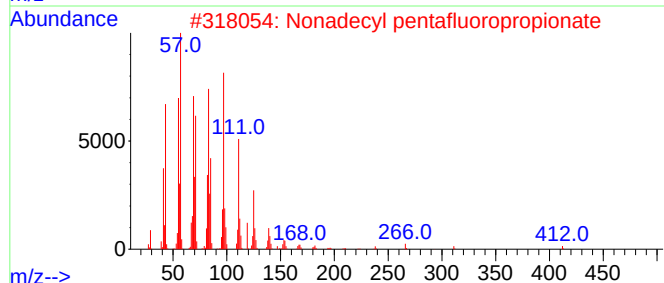
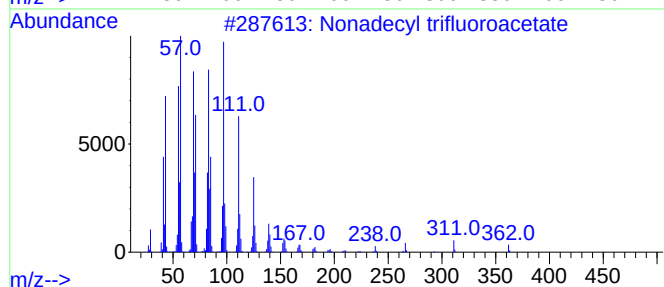
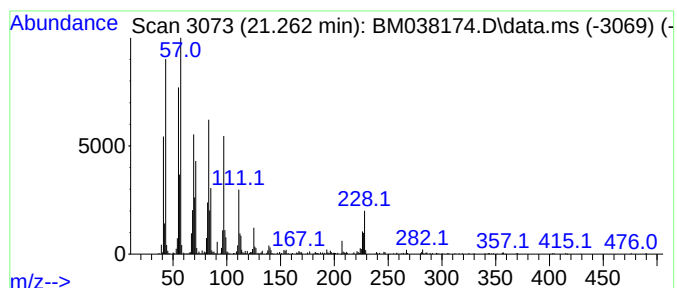
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Nonadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.262	5.83 ng/ul	653231	Chrysene-d12	21.580

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	81
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	81
3			Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	81
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	81
5			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	81



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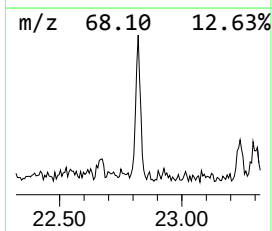
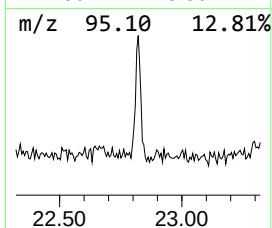
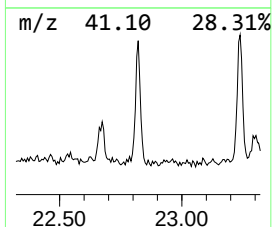
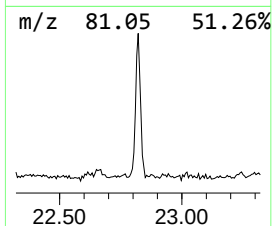
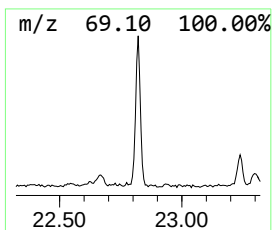
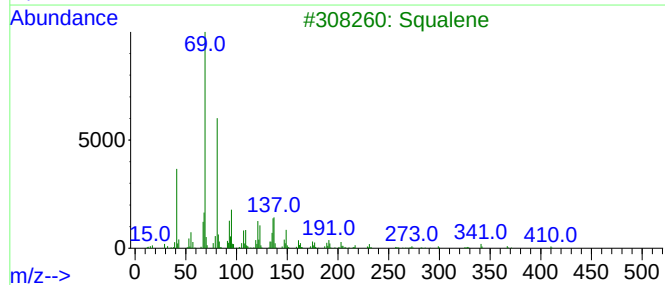
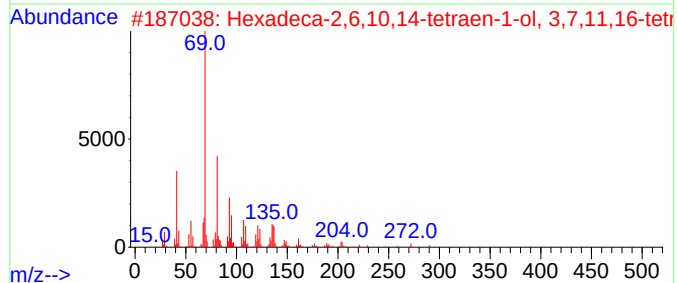
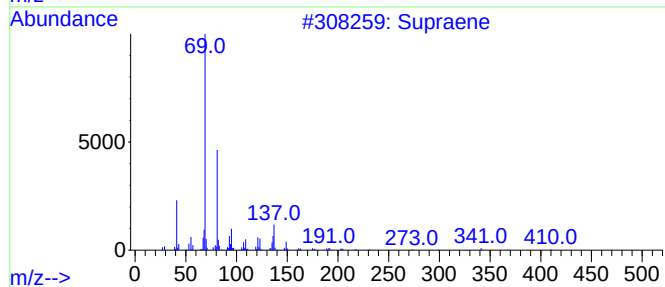
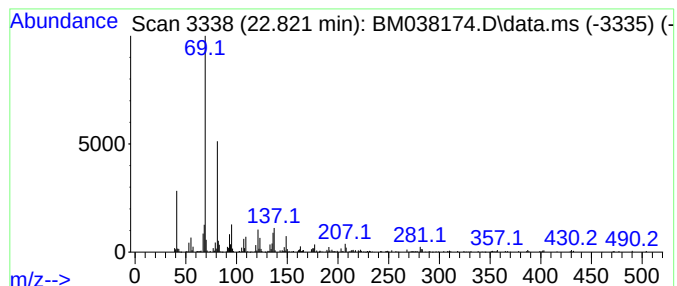
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.821	2.77 ng/ul	265691	Perylene-d12	24.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	80
3			Squalene	410	C30H50	000111-02-4	80
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038174.D
Acq On : 21 Dec 2022 16:25
Operator : CG/JU
Sample : N6014-21
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXT3

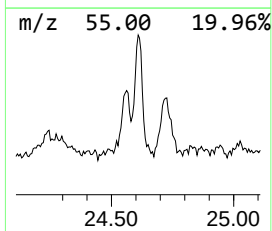
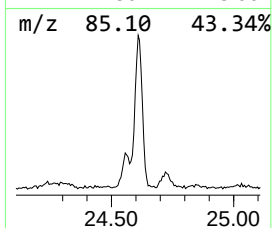
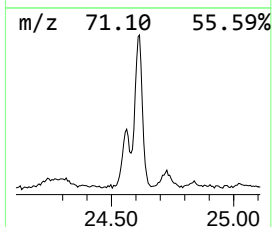
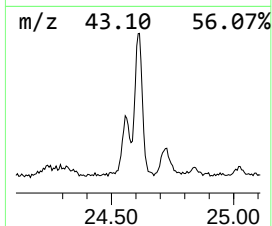
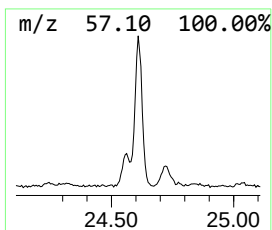
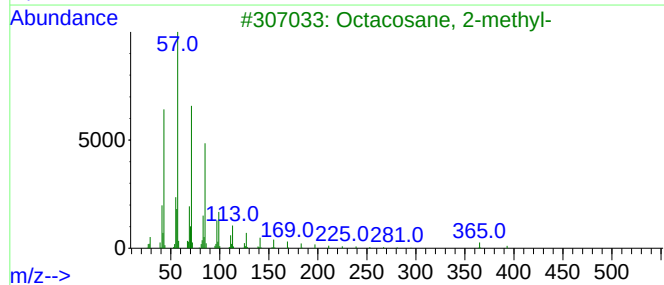
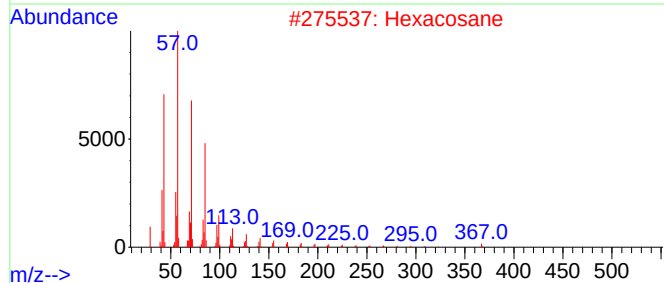
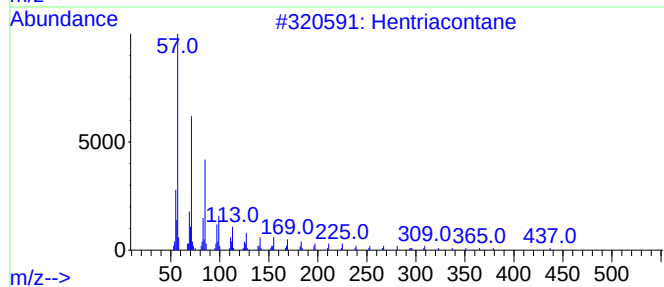
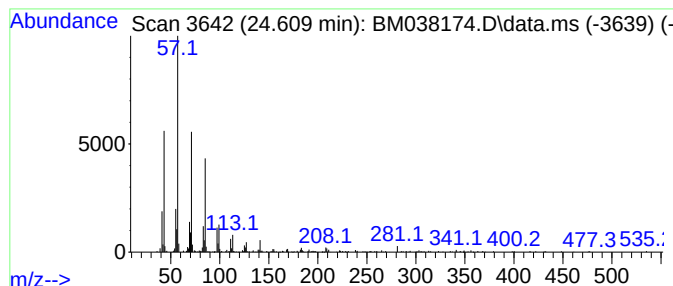
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.609	6.97 ng/ul	667710	Perylene-d12	24.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	87
2			Hexacosane	366	C26H54	000630-01-3	87
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	86
4			Octacosane	394	C28H58	000630-02-4	86
5			Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038174.D
Acq On : 21 Dec 2022 16:25
Operator : CG/JU
Sample : N6014-21
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXT3

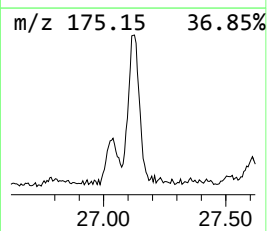
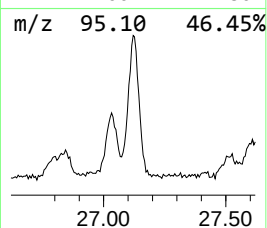
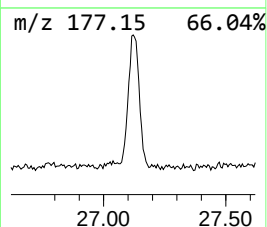
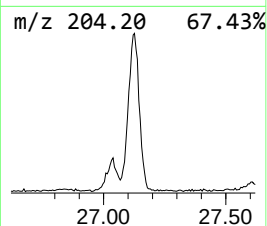
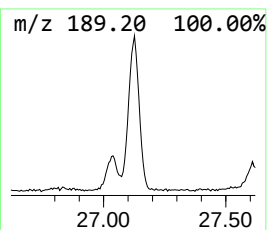
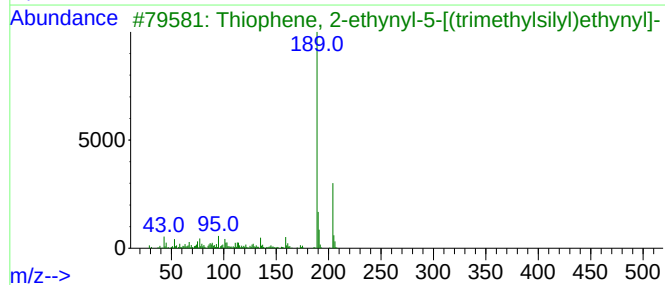
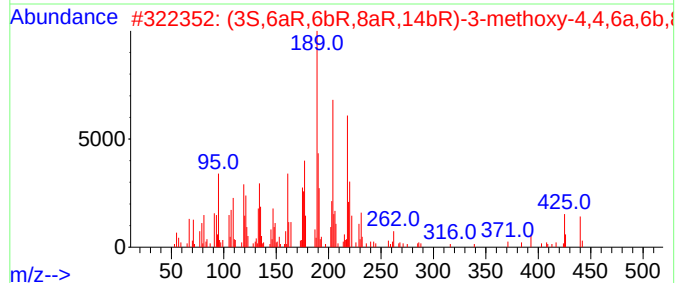
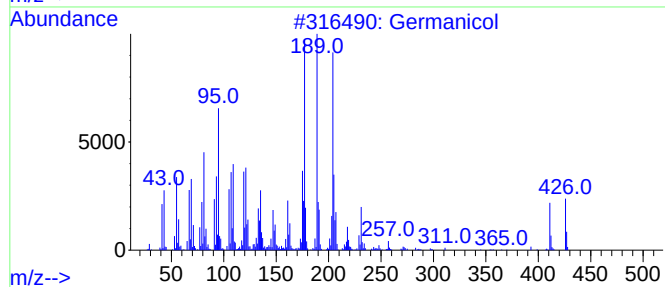
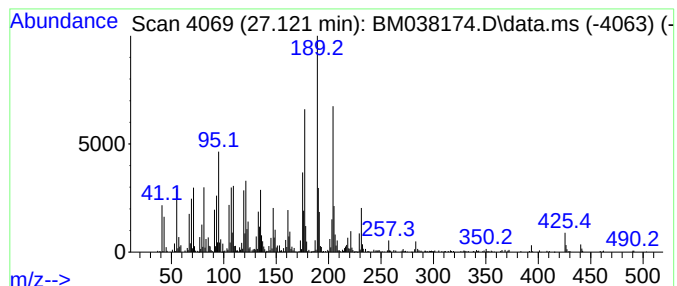
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Germanicol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.121	18.44 ng/ul	1766900	Perylene-d12	24.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Germanicol	426	C30H50O	000465-02-1	64
2			(3S,6aR,6bR,8aR,14bR)-3-methoxy-...	440	C31H52O	1000441-97-8	58
3			Thiophene, 2-ethynyl-5-[(trimeth...	204	C11H12SSi	182323-29-1	47
4			2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	46
5			4a,8-Dimethyl-2-(prop-1-en-2-yl)...	204	C15H24	103827-22-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038174.D
Acq On : 21 Dec 2022 16:25
Operator : CG/JU
Sample : N6014-21
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXT3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.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 ...	18.286	8.7	ng/ul	1095350	4	17.410	2533830	20.0
Octadecanoic acid	19.551	2.1	ng/ul	237205	5	21.580	2241730	20.0
Nonadecyl trifl...	21.262	5.8	ng/ul	653231	5	21.580	2241730	20.0
Supraene	22.821	2.8	ng/ul	265691	6	24.033	1916320	20.0
(DEL) Alkane: S...	24.609	7.0	ng/ul	667710	6	24.033	1916320	20.0
Germanicol	27.121	18.4	ng/ul	1766900	6	24.033	1916320	20.0