

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022824\
 Data File : BM044441.D
 Acq On : 29 Feb 2024 16:03
 Operator : MA/JU
 Sample : P1512-10
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 E0SC3

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-BM022324.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM044441.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.369	44	48	57	rVB	79565	102787	1.76%	0.159%
2	3.669	97	99	104	rVB	8568	11358	0.19%	0.018%
3	3.787	115	119	136	rBV	911101	1444906	24.68%	2.229%
4	4.110	171	174	180	rVB	16683	24598	0.42%	0.038%
5	4.340	209	213	221	rVB2	28386	42264	0.72%	0.065%
6	4.752	280	283	289	rBV7	10158	17698	0.30%	0.027%
7	6.046	499	503	504	rBV3	7176	7746	0.13%	0.012%
8	6.946	651	656	659	rBV7	9791	16913	0.29%	0.026%
9	7.116	678	685	697	rBV	1117508	1812606	30.96%	2.796%
10	7.298	710	716	726	rVB	913812	1487047	25.40%	2.294%
11	7.481	740	747	757	rBV	1081312	1779485	30.40%	2.745%
12	7.598	763	767	771	rBV6	4726	10536	0.18%	0.016%
13	7.651	774	776	783	rVB7	4422	6616	0.11%	0.010%
14	7.951	820	827	835	rBV	632265	995687	17.01%	1.536%
15	8.016	835	838	842	rBV2	15195	21729	0.37%	0.034%
16	8.669	940	949	955	rBV	1353825	2219712	37.92%	3.424%
17	8.722	955	958	968	rVB	116384	189323	3.23%	0.292%
18	9.128	1019	1027	1036	rBV	993816	1690536	28.88%	2.608%
19	9.228	1041	1044	1049	rVV7	7403	12072	0.21%	0.019%
20	9.292	1051	1055	1060	rVB8	10899	18663	0.32%	0.029%
21	9.716	1122	1127	1136	rVB8	7698	19343	0.33%	0.030%
22	9.845	1141	1149	1159	rBV	827501	1391153	23.76%	2.146%
23	10.092	1187	1191	1195	rBV7	4405	7321	0.13%	0.011%
24	10.381	1233	1240	1254	rBV	1270043	2163671	36.96%	3.338%
25	10.757	1296	1304	1311	rBV	860541	1463438	25.00%	2.258%
26	10.810	1311	1313	1319	rVB	9277	11094	0.19%	0.017%
27	10.910	1320	1330	1345	rBV	1175479	2188084	37.38%	3.376%
28	11.528	1431	1435	1439	rBV4	9028	15421	0.26%	0.024%
29	12.186	1541	1547	1552	rBV6	8050	15912	0.27%	0.025%
30	12.280	1555	1563	1567	rBV9	6971	18145	0.31%	0.028%
31	12.351	1569	1575	1581	rVB2	25788	45257	0.77%	0.070%
32	12.422	1583	1587	1592	rBV7	4107	8273	0.14%	0.013%
33	12.628	1615	1622	1625	rBV9	3283	7815	0.13%	0.012%
34	12.886	1663	1666	1670	rVB6	4847	6502	0.11%	0.010%
35	13.133	1702	1708	1712	rBV7	5553	10676	0.18%	0.016%
36	13.427	1754	1758	1760	rBV4	11587	17001	0.29%	0.026%

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37	13.463	1760	1764	1766	rVV	20604	33674	0.58%	0.052%
38	13.504	1766	1771	1778	rVV	64123	114373	1.95%	0.176%
39	13.575	1778	1783	1789	rVB10	8504	18380	0.31%	0.028%
40	14.016	1850	1858	1866	rBV	2112291	3019893	51.59%	4.659%
41	14.286	1896	1904	1916	rBV	2619966	3912715	66.84%	6.036%
42	14.427	1923	1928	1932	rVB8	9014	12119	0.21%	0.019%
43	14.504	1937	1941	1945	rVB5	10481	16536	0.28%	0.026%
44	14.592	1949	1956	1964	rBV	1241208	1815926	31.02%	2.801%
45	14.663	1964	1968	1971	rVB6	6029	9001	0.15%	0.014%
46	14.804	1984	1992	2018	rBV	557905	1304214	22.28%	2.012%
47	15.010	2025	2027	2035	rVB9	14594	27469	0.47%	0.042%
48	15.151	2041	2051	2063	rVB	76223	168304	2.87%	0.260%
49	15.451	2099	2102	2106	rVB3	9353	13667	0.23%	0.021%
50	15.586	2118	2125	2134	rBV	3295490	4692149	80.15%	7.239%
51	15.710	2140	2146	2159	rBV	797887	1131730	19.33%	1.746%
52	15.833	2163	2167	2169	rBV5	11689	15502	0.26%	0.024%
53	16.239	2232	2236	2244	rBV3	19106	27140	0.46%	0.042%
54	16.316	2245	2249	2255	rVV6	17320	39151	0.67%	0.060%
55	16.374	2255	2259	2263	rVB7	16312	22056	0.38%	0.034%
56	16.651	2304	2306	2311	rVV6	4425	6015	0.10%	0.009%
57	16.751	2317	2323	2329	rBV6	19467	36212	0.62%	0.056%
58	17.015	2366	2368	2374	rVB7	7809	9685	0.17%	0.015%
59	17.110	2381	2384	2390	rBV6	22733	36007	0.62%	0.056%
60	17.339	2416	2423	2429	rBV	1444868	2099754	35.87%	3.239%
61	17.386	2429	2431	2434	rVV	42886	54045	0.92%	0.083%
62	17.439	2434	2440	2450	rVB2	3298161	4853958	82.91%	7.488%
63	17.739	2485	2491	2499	rBV5	43760	102285	1.75%	0.158%
64	18.127	2553	2557	2561	rBV7	12643	22537	0.38%	0.035%
65	18.251	2573	2578	2587	rBV	420235	630246	10.77%	0.972%
66	18.686	2648	2652	2655	rBV	93736	106907	1.83%	0.165%
67	18.721	2655	2658	2665	rVB6	36747	51884	0.89%	0.080%
68	19.304	2753	2757	2761	rVB2	52430	72792	1.24%	0.112%
69	19.368	2765	2768	2770	rBV	38465	49842	0.85%	0.077%
70	19.404	2770	2774	2779	rVB	153901	215942	3.69%	0.333%
71	19.533	2792	2796	2803	rBV	111627	147131	2.51%	0.227%
72	19.733	2824	2830	2840	rBV	4086528	5854180	100.00%	9.031%
73	20.303	2924	2927	2932	rBV	55460	59136	1.01%	0.091%
74	20.756	3000	3004	3009	rBV	3224345	3451995	58.97%	5.325%
75	20.798	3009	3011	3016	rVB2	61465	68552	1.17%	0.106%
76	21.268	3087	3091	3098	rBV	269699	374046	6.39%	0.577%

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77	21.533	3131	3136	3141	rBV	1613669	2174965	37.15%	3.355%
78	22.186	3244	3247	3258	rVB	176743	289586	4.95%	0.447%
79	23.268	3427	3431	3436	rVB	252191	394961	6.75%	0.609%
80	23.803	3515	3522	3535	rBV2	2681885	5427182	92.71%	8.373%
81	23.956	3543	3548	3564	rVB	1143044	2536159	43.32%	3.913%

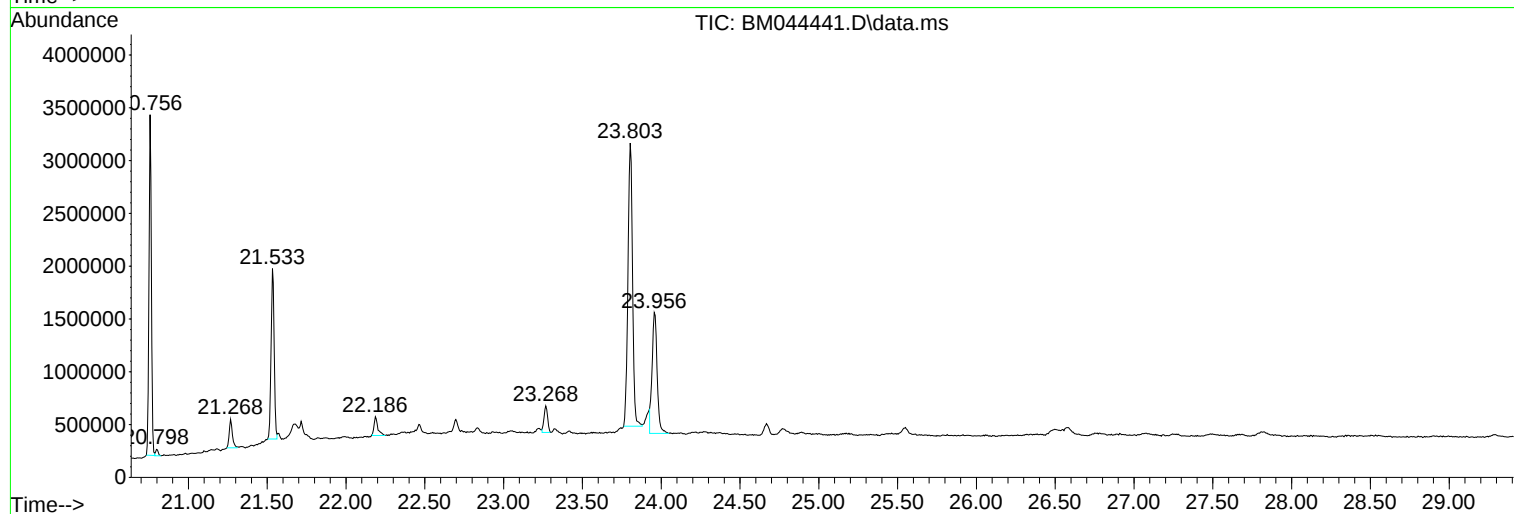
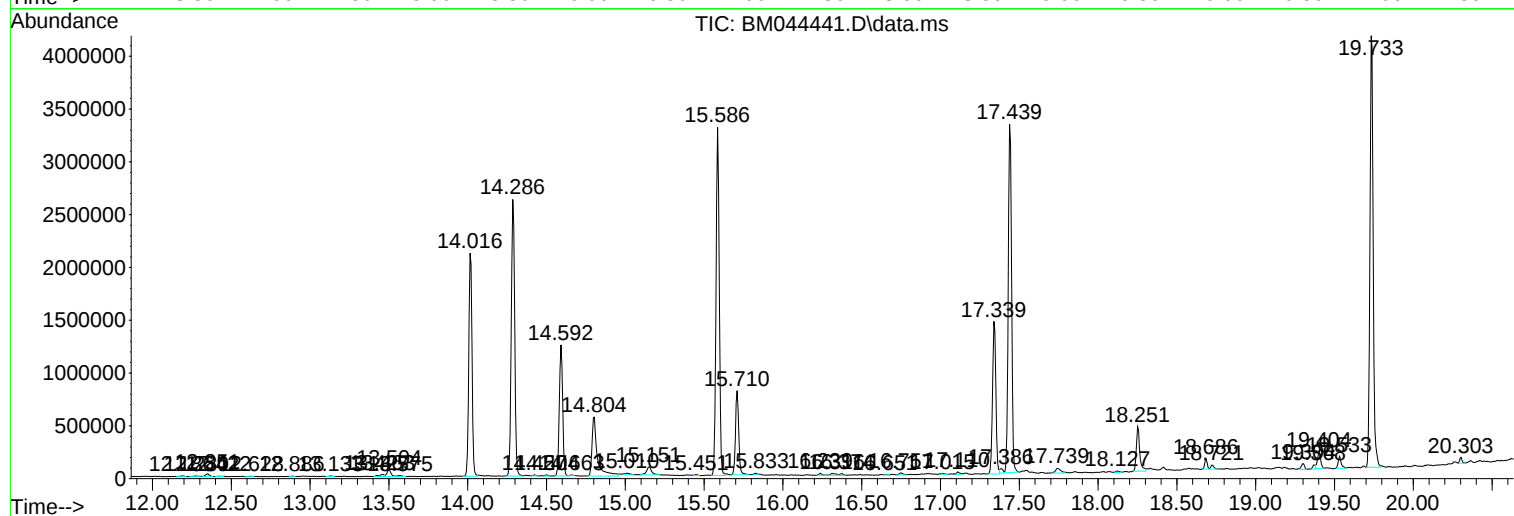
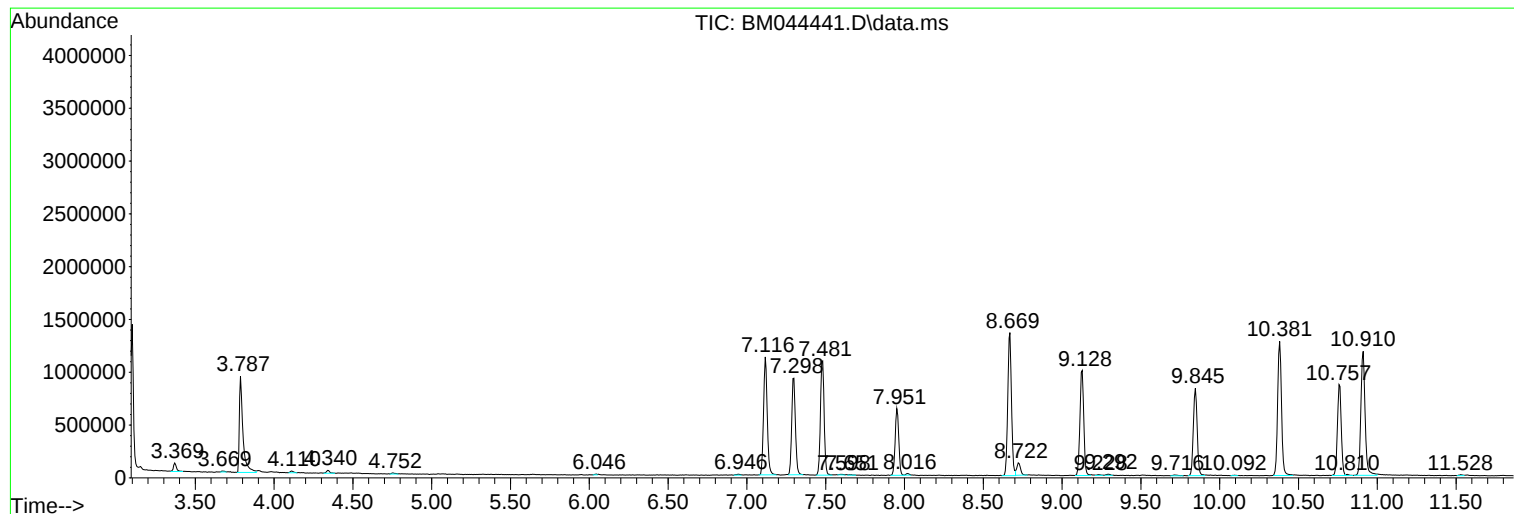
Sum of corrected areas: 64821391

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM022324.MA.M
Quant Title : SVOA CALIBRATION

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



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Operator : MA/JU
Sample : P1512-10
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Instrument :
BNA_M
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E0SC3

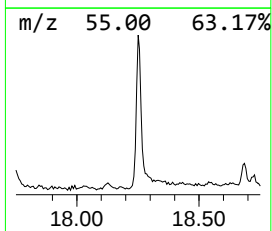
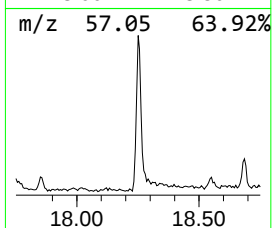
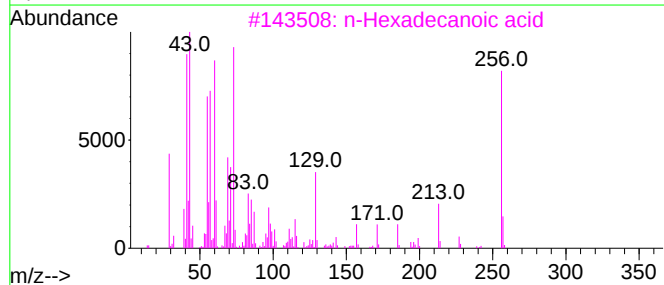
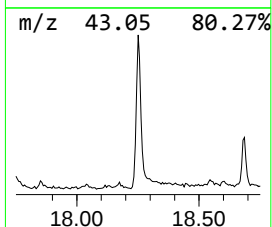
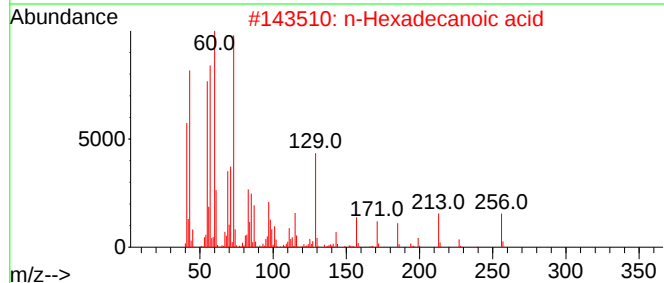
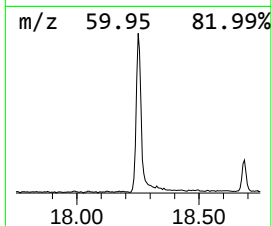
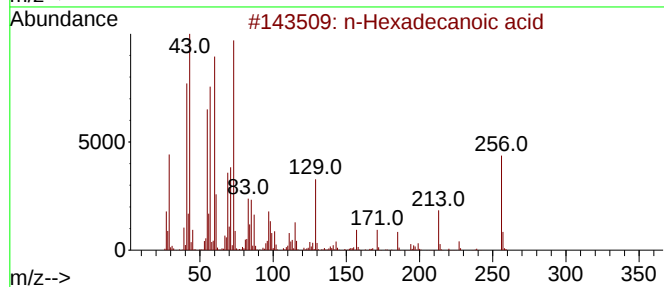
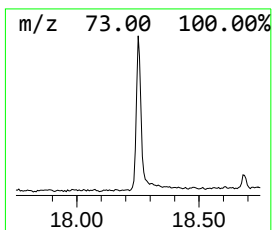
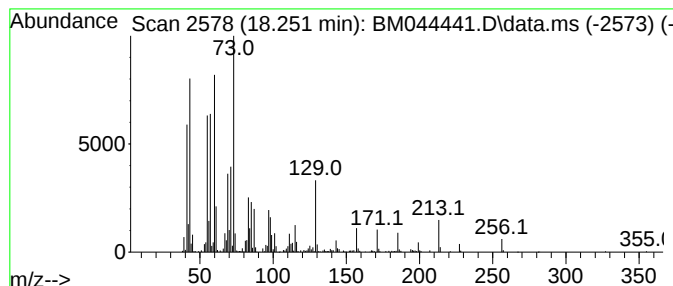
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM022324.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.251	6.00 ng/ul	630246	Phenanthrene-d10	17.339

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	98
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	87



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Sample : P1512-10
Misc :
ALS Vial : 41 Sample Multiplier: 1

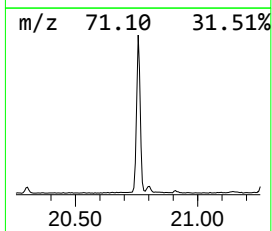
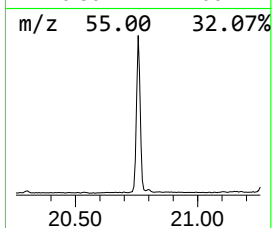
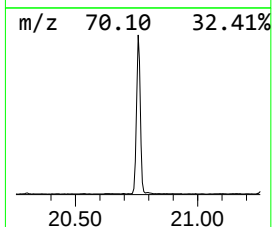
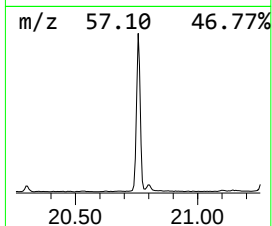
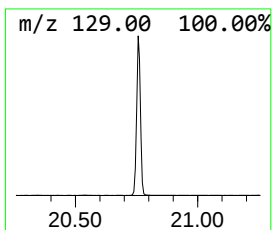
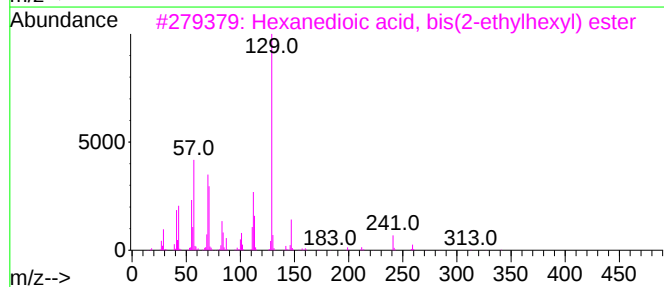
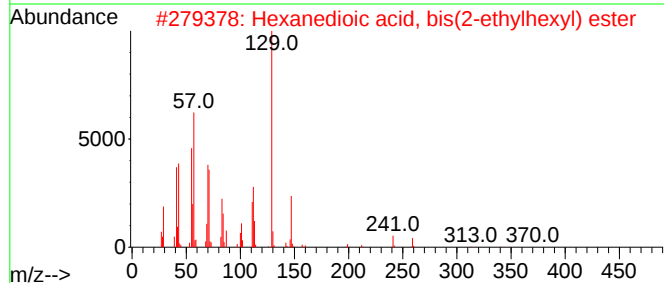
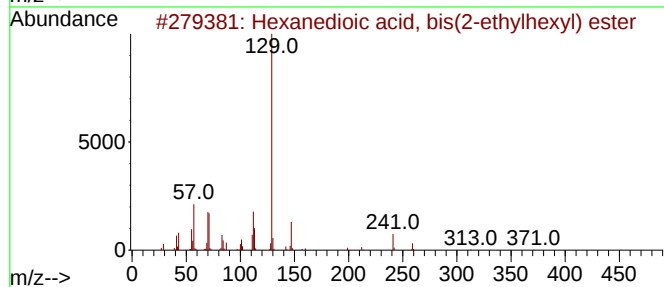
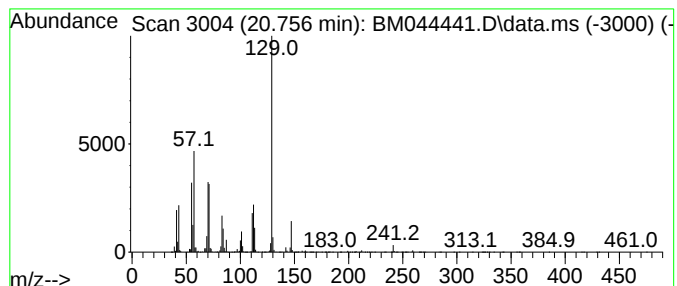
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Hexanedioic acid, bis(2-eth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.756	31.74 ng/ul	3452000	Chrysene-d12	21.533	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	91
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
3	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
4	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
5	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	81



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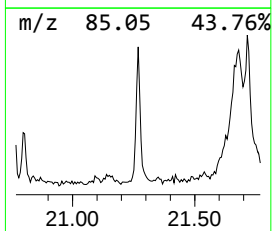
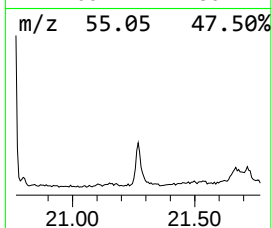
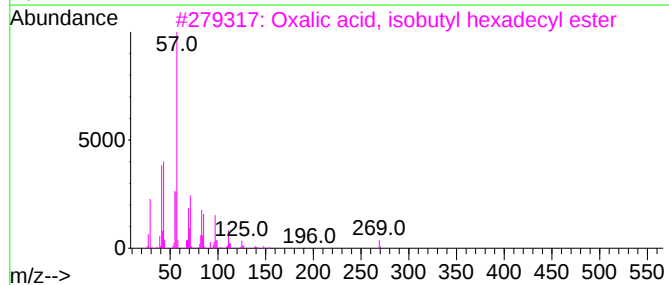
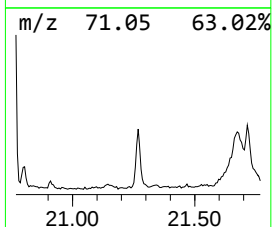
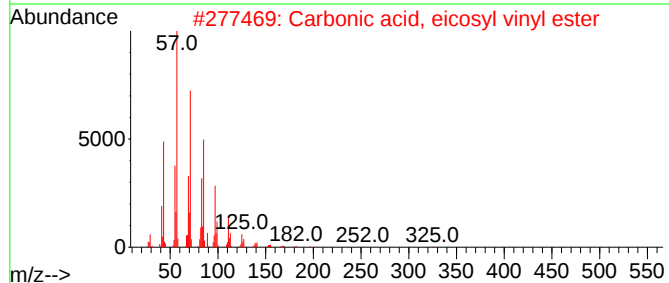
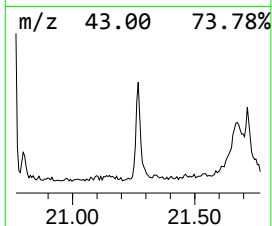
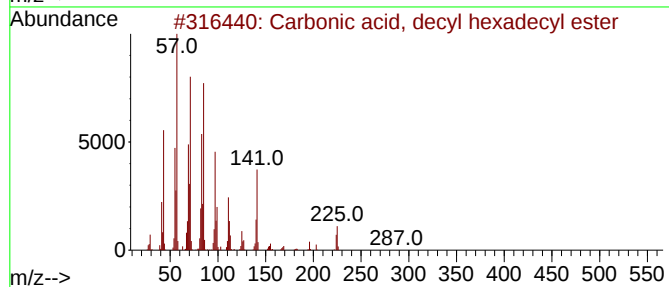
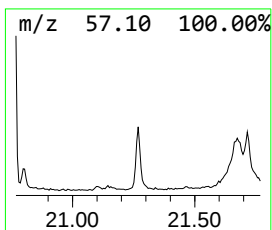
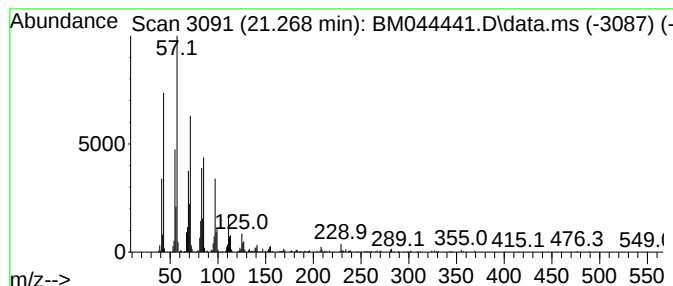
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Carbonic acid, decyl hexade... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.268	3.44 ng/ul	374046	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, decyl hexadecyl e...	426	C27H54O3	1000383-16-5	91
2			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	90
4			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	87



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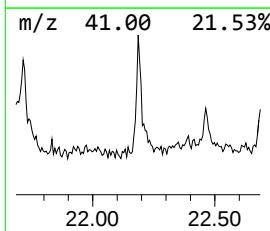
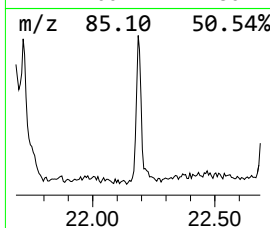
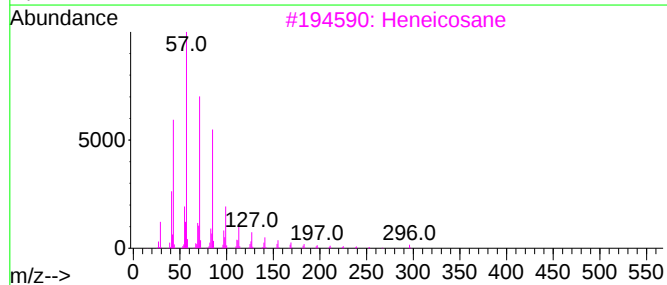
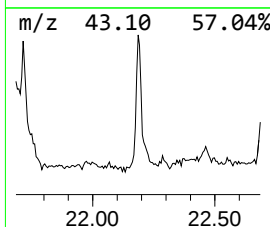
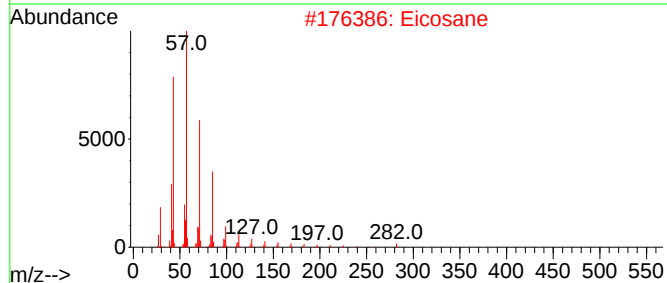
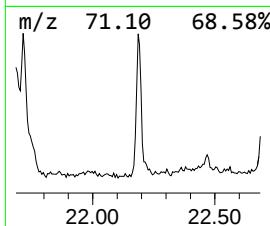
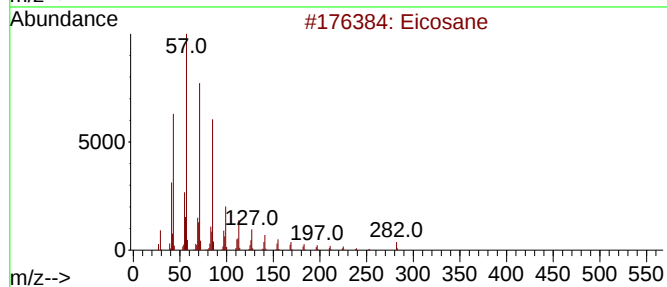
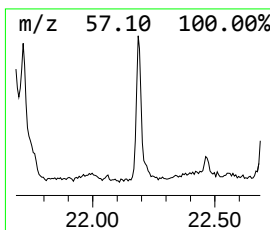
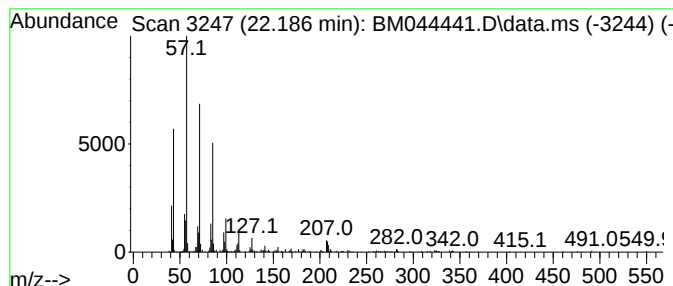
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.186	2.66 ng/ul	289586	Chrysene-d12	21.533

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	93
2		Eicosane	282	C20H42	000112-95-8	86
3		Heneicosane	296	C21H44	000629-94-7	83
4		Nonadecane	268	C19H40	000629-92-5	80
5		Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022824\
Data File : BM044441.D
Acq On : 29 Feb 2024 16:03
Operator : MA/JU
Sample : P1512-10
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0SC3

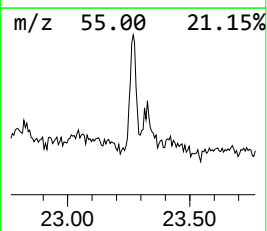
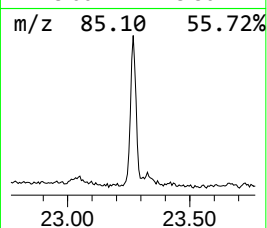
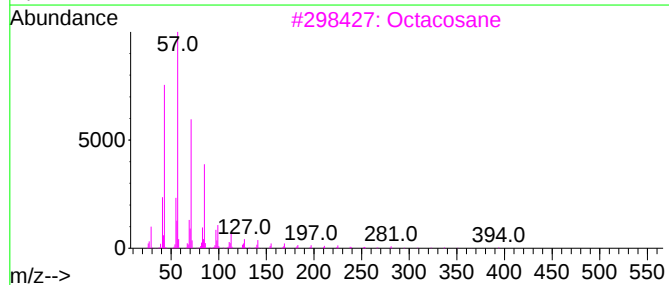
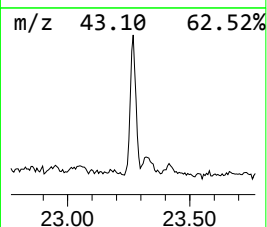
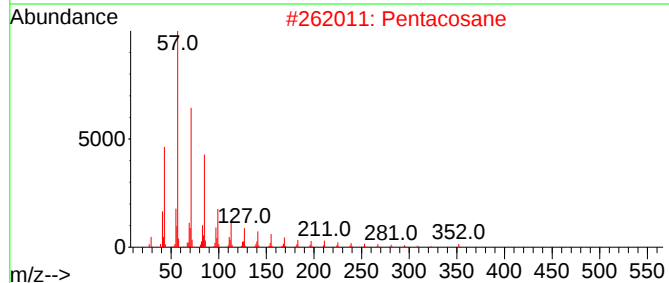
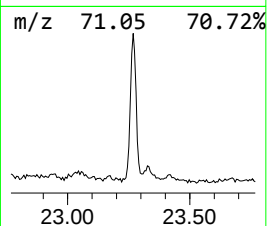
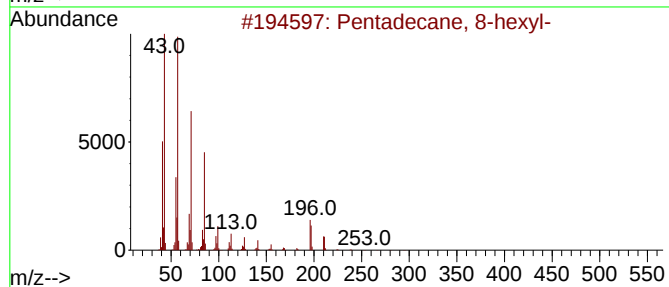
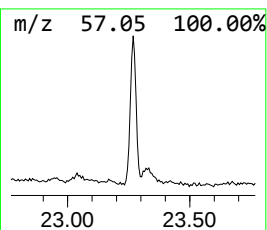
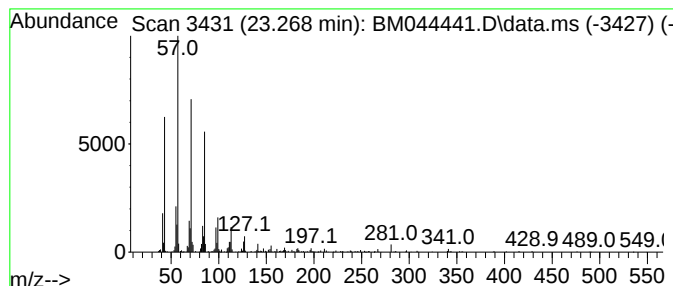
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.268	3.11 ng/ul	394961	Perylene-d12	23.956

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2		Pentacosane	352	C25H52	000629-99-2	90
3		Octacosane	394	C28H58	000630-02-4	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022824\
Data File : BM044441.D
Acq On : 29 Feb 2024 16:03
Operator : MA/JU
Sample : P1512-10
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0SC3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM022324.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 ...	18.251	6.0	ng/ul	630246	4	17.339	2099750	20.0
Hexanedioic aci...	20.756	31.7	ng/ul	3452000	5	21.533	2174970	20.0
Carbonic acid, ...	21.268	3.4	ng/ul	374046	5	21.533	2174970	20.0
(DEL) Alkane: S...	22.186	2.7	ng/ul	289586	5	21.533	2174970	20.0
(DEL) Alkane: S...	23.268	3.1	ng/ul	394961	6	23.956	2536160	20.0