

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081823\
 Data File : BP016648.D
 Acq On : 18 Aug 2023 19:13
 Operator : MA/JU
 Sample : 03968-26
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A48P3

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-BP081423.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP016648.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.393	14	18	30	rVB	91887	139513	1.90%	0.169%
2	3.828	88	92	108	rBV	577991	902484	12.27%	1.095%
3	3.946	108	112	115	rVB3	15341	17880	0.24%	0.022%
4	4.034	122	127	134	rVB	76576	127695	1.74%	0.155%
5	4.146	143	146	155	rVB	20451	38060	0.52%	0.046%
6	4.311	170	174	177	rVB6	5320	7521	0.10%	0.009%
7	4.540	209	213	220	rBV7	16408	45072	0.61%	0.055%
8	4.734	242	246	252	rVB2	45711	62811	0.85%	0.076%
9	5.087	300	306	313	rBV	55005	88061	1.20%	0.107%
10	5.205	322	326	331	rVB5	11733	17516	0.24%	0.021%
11	5.675	401	406	412	rVB2	20913	44251	0.60%	0.054%
12	5.993	457	460	463	rBV5	4672	7916	0.11%	0.010%
13	6.493	540	545	553	rBV2	20823	45072	0.61%	0.055%
14	6.834	599	603	607	rBV7	4593	9058	0.12%	0.011%
15	6.993	626	630	631	rBV4	8295	9349	0.13%	0.011%
16	7.193	657	664	676	rVB	1164340	1934833	26.31%	2.347%
17	7.387	689	697	706	rBV	970867	1497151	20.36%	1.816%
18	7.569	720	728	736	rBV	1150049	1810894	24.63%	2.197%
19	7.640	736	740	751	rVB	85315	146485	1.99%	0.178%
20	7.852	773	776	781	rVB4	7477	10502	0.14%	0.013%
21	8.052	801	810	820	rBV	1173126	1865453	25.37%	2.263%
22	8.387	862	867	875	rBV3	14229	35018	0.48%	0.042%
23	8.752	922	929	940	rBV	1439441	2305660	31.36%	2.797%
24	8.840	942	944	948	rVV4	14470	25866	0.35%	0.031%
25	8.899	948	954	963	rVB	131906	221333	3.01%	0.268%
26	9.246	1004	1013	1025	rBV	1152076	1882414	25.60%	2.284%
27	9.475	1049	1052	1056	rBV5	8420	13669	0.19%	0.017%
28	9.963	1126	1135	1144	rBV	899117	1508987	20.52%	1.831%
29	10.075	1150	1154	1162	rBV	23667	41061	0.56%	0.050%
30	10.328	1192	1197	1201	rBV5	11741	21216	0.29%	0.026%
31	10.487	1217	1224	1239	rBV	1421005	2389350	32.50%	2.898%
32	10.640	1244	1250	1253	rVV8	5926	11538	0.16%	0.014%
33	10.881	1283	1291	1300	rBV	1747214	2925906	39.79%	3.549%
34	11.034	1309	1317	1334	rBV	1165620	2070749	28.16%	2.512%
35	11.428	1378	1384	1391	rVB10	10484	27222	0.37%	0.033%
36	11.569	1403	1408	1410	rBV6	7173	10420	0.14%	0.013%

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Max Peaks: 100

Stop Thrs : 0

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP081423.MA.M
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37	11.622	1414	1417	1425	rVV9	7543	16595	0.23%	0.020%
38	11.693	1425	1429	1434	rVB7	8759	15102	0.21%	0.018%
39	11.799	1442	1447	1453	rBV10	5752	11140	0.15%	0.014%
40	11.905	1459	1465	1472	rVB10	7129	15377	0.21%	0.019%
41	12.269	1523	1527	1534	rVV7	12792	23374	0.32%	0.028%
42	12.352	1536	1541	1544	rBV7	6680	9288	0.13%	0.011%
43	12.457	1552	1559	1566	rBV2	27245	47927	0.65%	0.058%
44	13.034	1653	1657	1661	rVB6	5397	9507	0.13%	0.012%
45	13.463	1726	1730	1738	rBV8	12204	22053	0.30%	0.027%
46	13.551	1738	1745	1750	rVV	103896	167119	2.27%	0.203%
47	13.640	1756	1760	1763	rBV6	7077	12880	0.18%	0.016%
48	13.887	1797	1802	1807	rVV4	17223	27073	0.37%	0.033%
49	14.022	1819	1825	1828	rBV7	12710	16800	0.23%	0.020%
50	14.110	1834	1840	1856	rBV	2812988	3803993	51.74%	4.615%
51	14.316	1869	1875	1882	rBV	10456	20744	0.28%	0.025%
52	14.398	1882	1889	1909	rBV	3024972	4566561	62.11%	5.540%
53	14.534	1910	1912	1916	rVB5	6747	7642	0.10%	0.009%
54	14.704	1934	1941	1949	rBV	2827493	4089093	55.61%	4.960%
55	14.904	1968	1975	1992	rBV	1180860	1973692	26.84%	2.394%
56	15.081	1999	2005	2009	rBV8	31915	62503	0.85%	0.076%
57	15.128	2009	2013	2023	rVB2	108038	168562	2.29%	0.204%
58	15.440	2064	2066	2071	rVB5	6337	8648	0.12%	0.010%
59	15.493	2071	2075	2076	rBV3	7947	8975	0.12%	0.011%
60	15.698	2102	2110	2120	rBV	3912713	5695795	77.46%	6.910%
61	15.816	2124	2130	2141	rVV	843111	1218005	16.57%	1.478%
62	15.934	2146	2150	2155	rVB5	17396	28992	0.39%	0.035%
63	16.422	2229	2233	2239	rVB2	25737	40592	0.55%	0.049%
64	16.822	2297	2301	2308	rVB9	13932	21677	0.29%	0.026%
65	16.975	2325	2327	2333	rBV7	6713	11427	0.16%	0.014%
66	17.469	2405	2411	2416	rBV	3609065	4968358	67.57%	6.027%
67	17.510	2416	2418	2422	rVV	81542	101144	1.38%	0.123%
68	17.569	2422	2428	2438	rVV2	4260790	6075673	82.63%	7.370%
69	17.645	2438	2441	2447	rVB5	42488	63683	0.87%	0.077%
70	18.087	2514	2516	2521	rVB5	20078	24325	0.33%	0.030%
71	18.310	2549	2554	2566	rBV	919728	1541554	20.97%	1.870%
72	19.122	2689	2692	2696	rBV2	34360	56790	0.77%	0.069%
73	19.375	2732	2735	2738	rBV	61473	67255	0.91%	0.082%
74	19.469	2748	2751	2755	rVB	190495	243126	3.31%	0.295%
75	19.539	2760	2763	2775	rBV	383052	638408	8.68%	0.774%
76	19.798	2802	2807	2818	rBV	5318826	7352776	100.00%	8.920%

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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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77	21.222	3045	3049	3056	rBV	1119194	1543016	20.99%	1.872%
78	21.563	3102	3107	3112	rBV	3442982	4835361	65.76%	5.866%
79	22.186	3209	3213	3220	rBV	634542	975757	13.27%	1.184%
80	23.980	3511	3518	3526	rVB2	2547258	5567040	75.71%	6.753%
81	24.151	3540	3547	3555	rVB	1903532	3940761	53.60%	4.780%

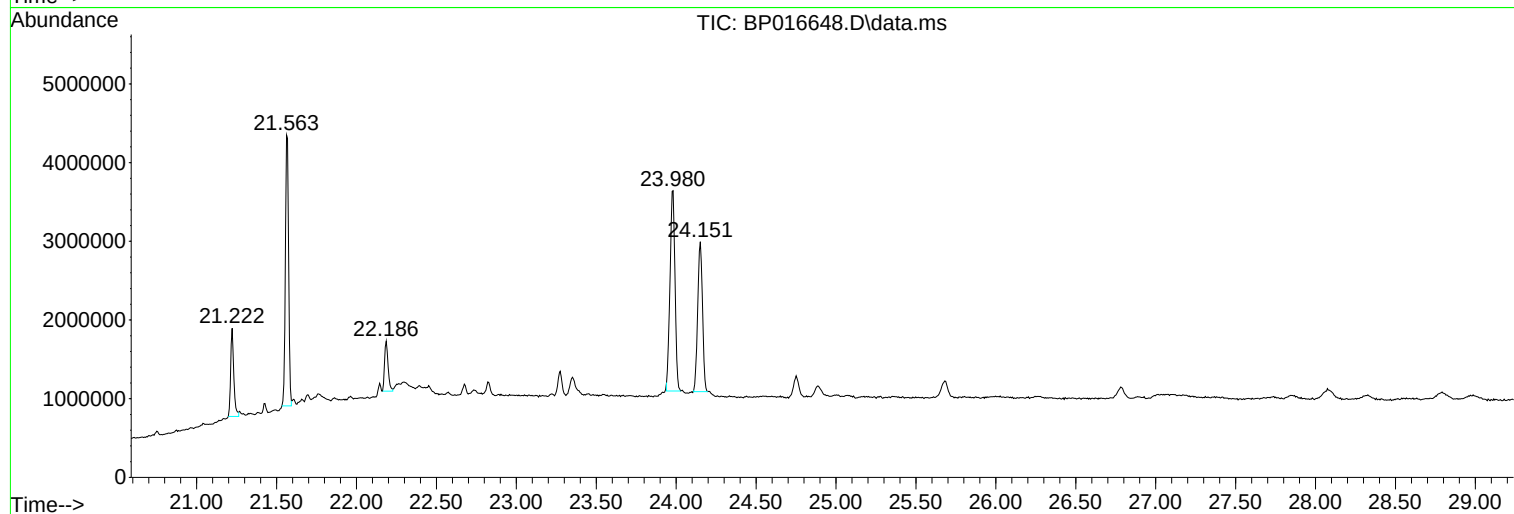
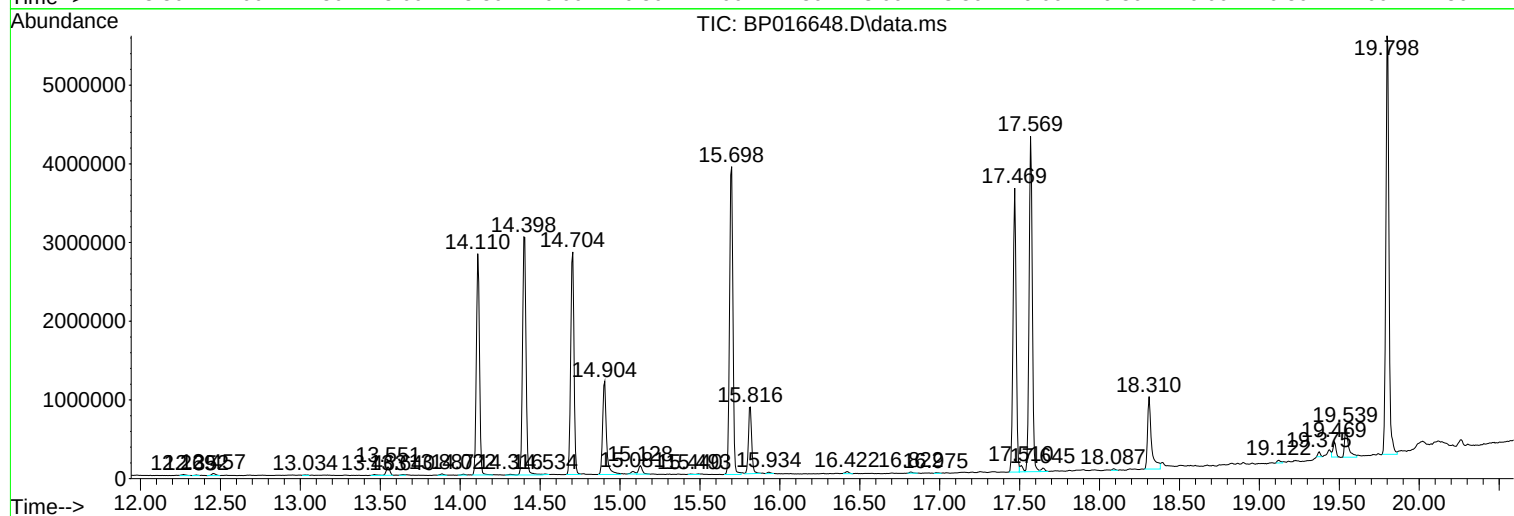
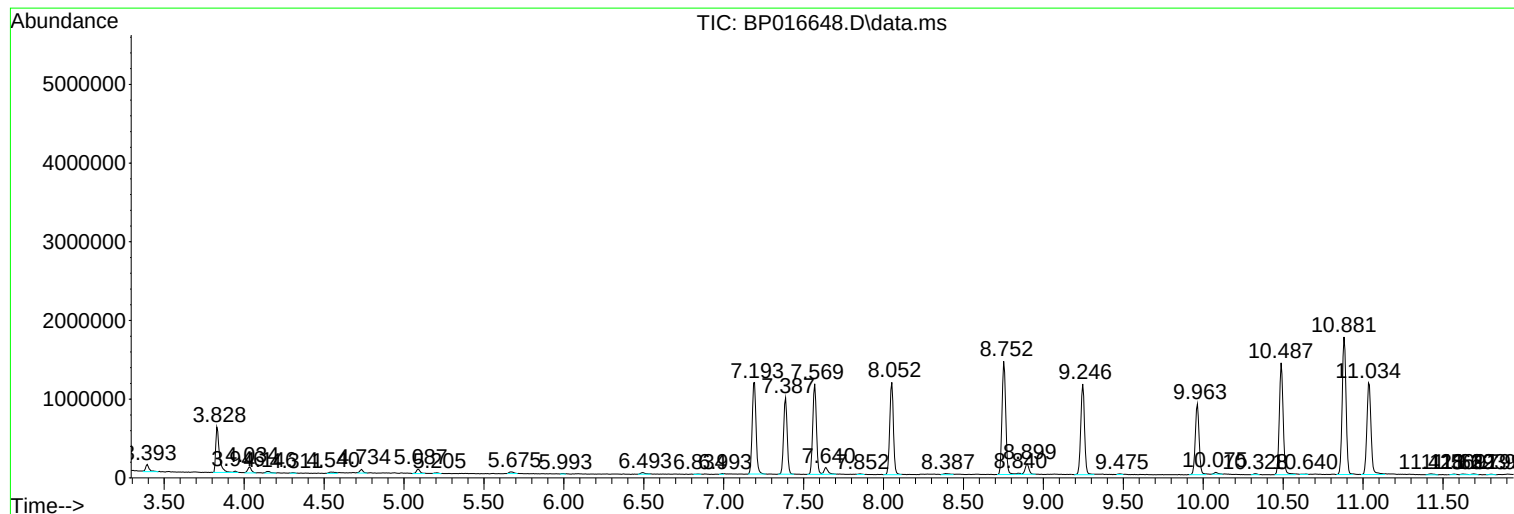
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP081423.MA.M
Quant Title : SVOA CALIBRATION

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



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Operator : MA/JU
Sample : 03968-26
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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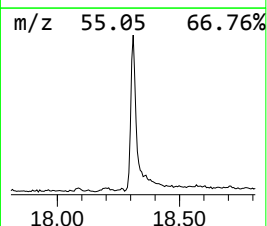
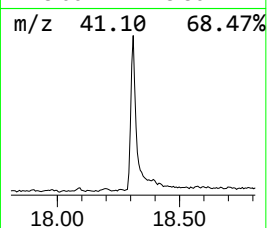
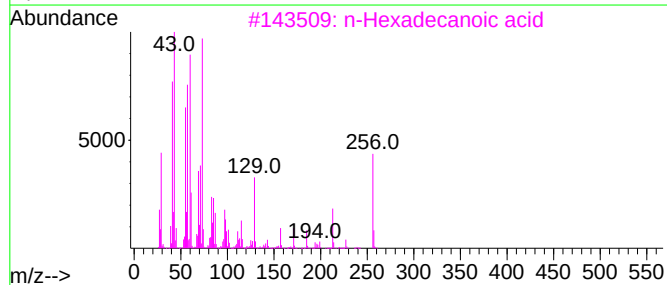
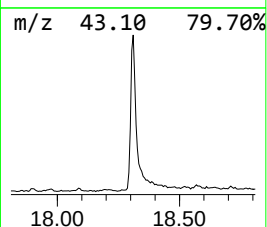
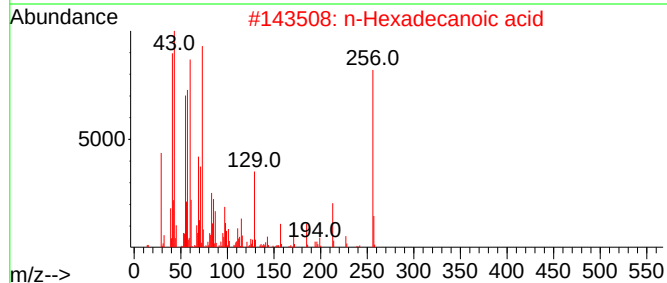
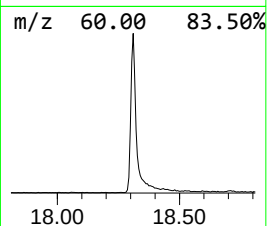
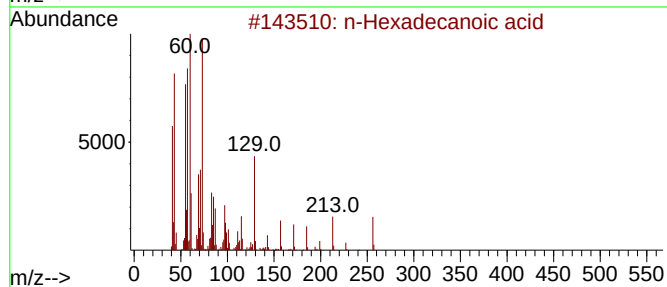
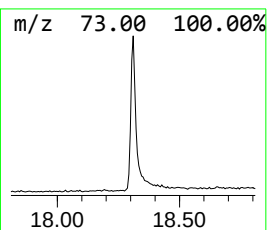
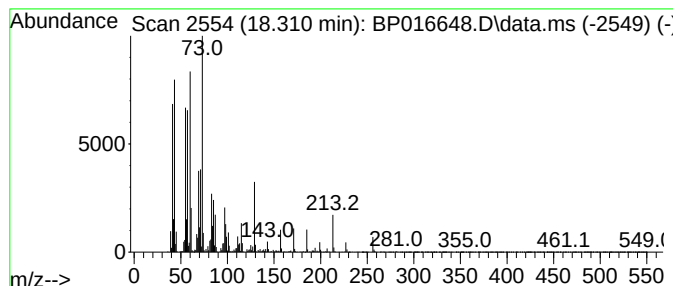
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP081423.MA.M
Quant Title : SVOA CALIBRATION

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.
18.310	6.21 ng/ul	1541550	Phenanthrene-d10	17.469

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	97
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	95



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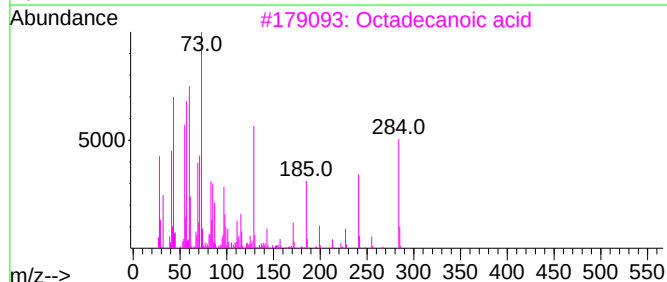
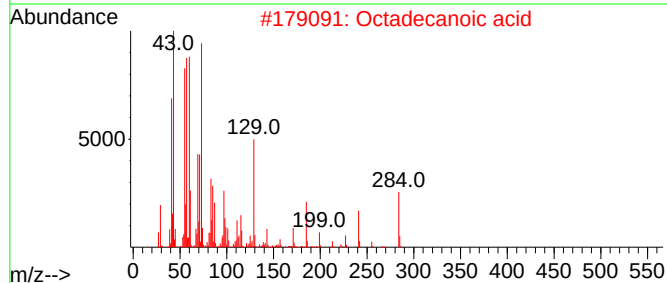
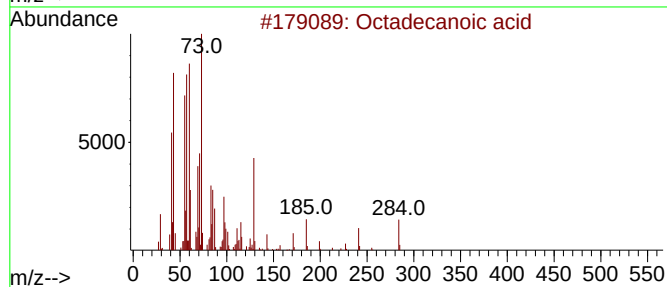
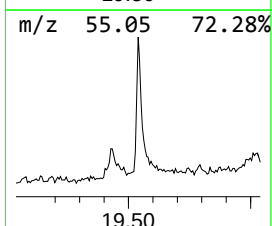
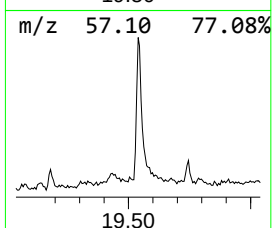
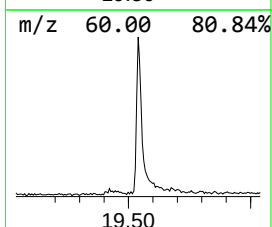
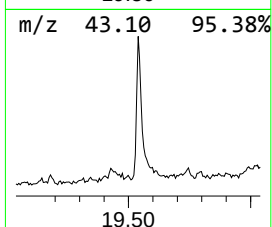
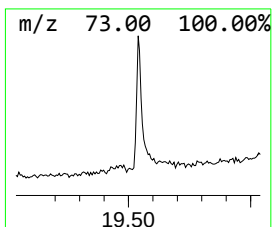
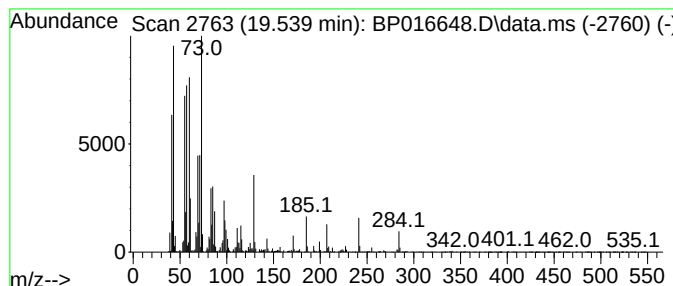
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP081423.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.539	2.64 ng/ul	638408	Chrysene-d12	21.563	
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	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	99
4	Octadecanoic acid	284	C18H36O2	000057-11-4	96
5	Octadecanoic acid	284	C18H36O2	000057-11-4	94



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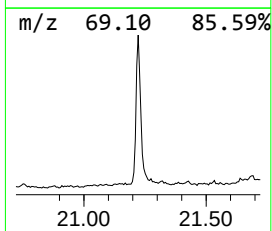
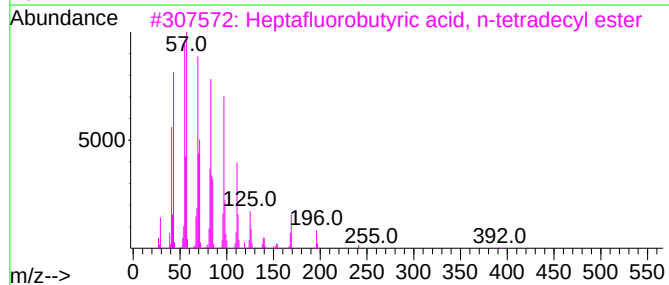
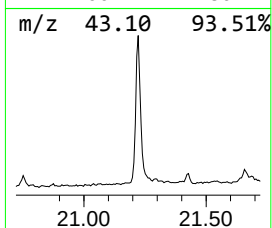
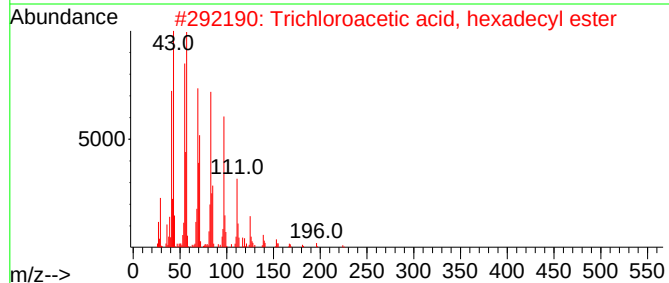
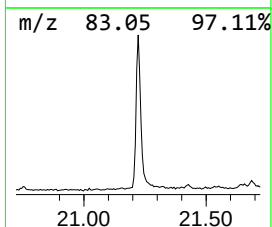
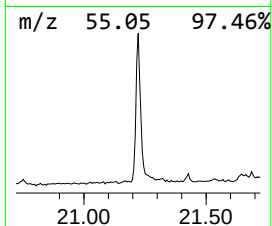
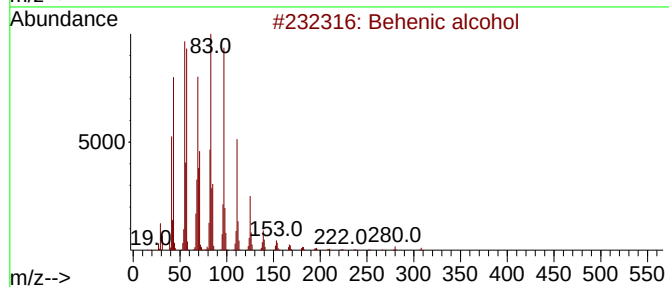
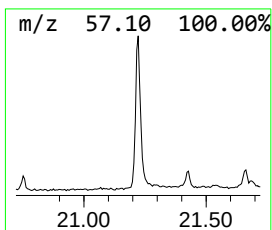
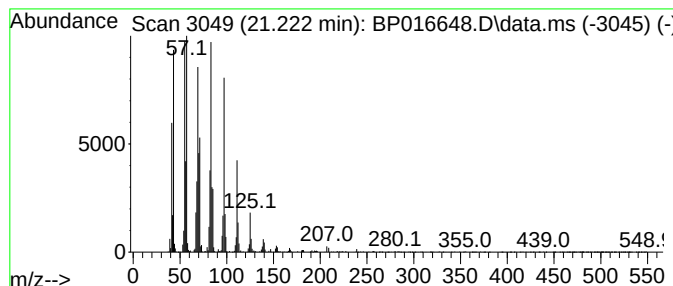
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP081423.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Behenic alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.222	6.38 ng/ul	1543020	Chrysene-d12	21.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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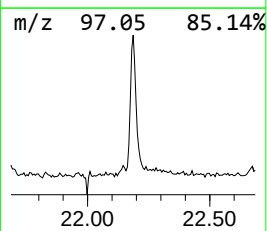
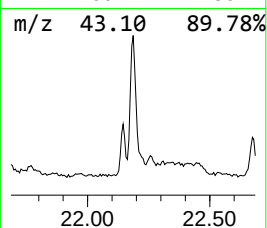
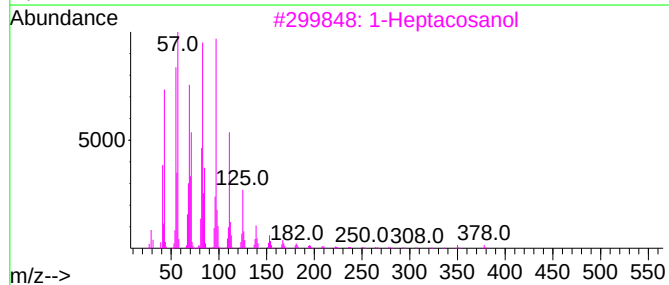
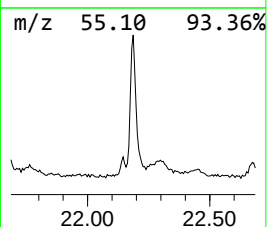
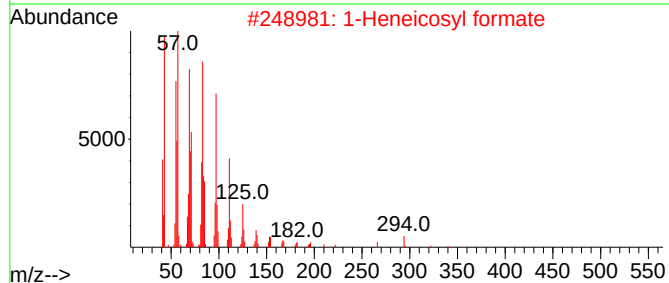
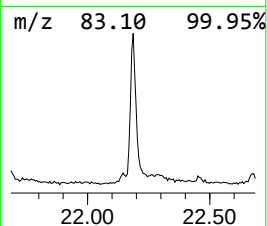
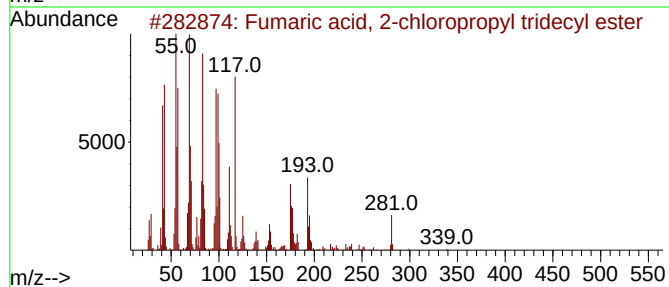
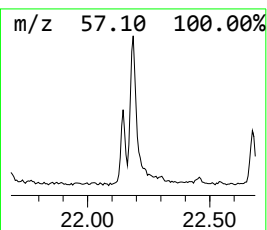
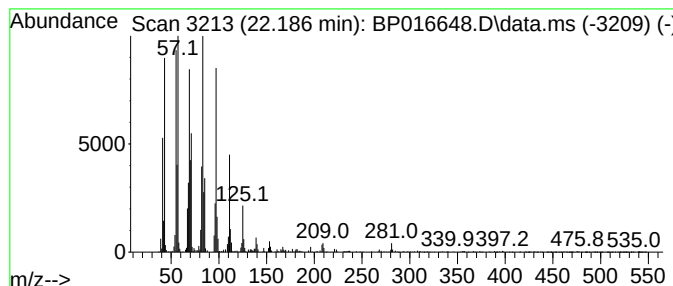
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Fumaric acid, 2-chloropropyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.186	4.04 ng/ul	975757	Chrysene-d12	21.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1010348-57-1	96
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
3			1-Heptacosanol	396	C27H56O	002004-39-9	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			Nonacos-1-ene	406	C29H58	018835-35-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081823\
Data File : BP016648.D
Acq On : 18 Aug 2023 19:13
Operator : MA/JU
Sample : 03968-26
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A48P3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP081423.MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.310	6.2	ng/ul	1541550	4	17.469	4968360	20.0
Octadecanoic acid	19.539	2.6	ng/ul	638408	5	21.563	4835360	20.0
Behenic alcohol	21.222	6.4	ng/ul	1543020	5	21.563	4835360	20.0
Fumaric acid, 2...	22.186	4.0	ng/ul	975757	5	21.563	4835360	20.0