LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016159.D
Acq On : 10 Jul 2023 15:16
Operator : MA/JU
Sample : 03404-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : YBW41

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-BP062623.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP016159.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.346	24	27	36	rVB2	38983	60113	1.13%	0.123%
2	3.805	103	105	120	rBV	176949	407734	7.70%	0.835%
3	4.528	226	228	235	rVB2	13224	21066	0.40%	0.043%
4	7.075	659	661	665	rVB5	5435	6045	0.11%	0.012%
5	7.246	683	690	705	rBV2	190828	791514	14.94%	1.621%
6	7.369	705	711	720	rVV	183531	425191	8.03%	0.871%
7	7.581	740	747	789	rVB	293227	964112	18.20%	1.974%
8	8.028	817	823	852	rBV	275407	1044627	19.72%	2.139%
9	8.810	949	956	994	rBV3	200392	1182793	22.33%	2.422%
10	9.257	1024	1032	1053	rBV	228007	870982	16.44%	1.784%
11	9.522	1074	1077	1084	rVB8	7628	15311	0.29%	0.031%
12	10.004	1149	1159	1193	rBV3	138962	859443	16.22%	1.760%
13	10.234	1195	1198	1199	rVV3	5992	6878	0.13%	0.014%
14	10.610	1253	1262	1277	rBV2	175648	878266	16.58%	1.798%
15	10.857	1297	1304	1328	rVB	542521	1753413	33.10%	3.590%
16	11.104	1337	1346	1376	rBV4	155836	955264	18.03%	1.956%
17	12.022	1498	1502	1507	rVB7	6479	9947	0.19%	0.020%
18	13.498	1748	1753	1754	rBV4	4003	5918	0.11%	0.012%
19	13.569	1760	1765	1775	rBV6	12866	34790	0.66%	0.071%
20	14.004	1835	1839	1841	rBV5	4763	5957	0.11%	0.012%
21	14.104	1848	1856	1880	rBV	830883	2356735	44.49%	4.826%
22	14.375	1895	1902	1928	rBV	1329404	2712470	51.20%	5.554%
23	14.675	1947	1953	1972	rVV	1339592	2615063	49.36%	5.355%
24	15.122	2018	2029	2031	rBV6	55190	155422	2.93%	0.318%
25	15.510	2091	2095	2097	rBV5	7170	8888	0.17%	0.018%
26	15.692	2118	2126	2149	rBV	1347637	3682118	69.50%	7.540%
27	15.922	2159	2165	2169	rBV4	98362	252572	4.77%	0.517%
28	16.081	2186	2192	2208	rVB	193650	413522	7.81%	0.847%
29	16.316	2230	2232	2236	rVB4	8104	9953	0.19%	0.020%
30	16.698	2292	2297	2298	rBV5	4503	6242	0.12%	0.013%
31	16.751	2304	2306	2310	rBV4	4512	5966	0.11%	0.012%
32	16.816	2315	2317	2321	rVV5	4753	5717	0.11%	0.012%
33	16.875	2325	2327	2332	rVV5	5645	8362	0.16%	0.017%
34	16.928	2332	2336	2338	rVB5	6028	8298	0.16%	0.017%
35	17.233	2386	2388	2393	rBV6	4453	6243	0.12%	0.013%
36	17.339	2402	2406	2407	rBV4	7862	8995	0.17%	0.018%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016159.D
Acq On : 10 Jul 2023 15:16
Operator : MA/JU
Sample : 03404-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YBW41

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-BP062623.MA.M
Title : SVOA CALIBRATION

37	17.439	2417	2423	2436	rBV	1862339	3216931	60.72%	6.587%
38	17.551	2436	2442	2474	rVB2	1217048	4084473	77.10%	8.364%
39	18.292	2563	2568	2580	rBV	168156	428424	8.09%	0.877%
40	18.680	2632	2634	2638	rVB5	12534	13311	0.25%	0.027%
41	19.357	2746	2749	2753	rBV2	34372	48814	0.92%	0.100%
42	19.527	2774	2778	2787	rBV4	65897	138629	2.62%	0.284%
43	19.780	2814	2821	2851	rBV	2136309	5297761	100.00%	10.848%
44	21.227	3063	3067	3076	rVB3	206345	497702	9.39%	1.019%
45	21.551	3117	3122	3131	rBV	1350013	3343797	63.12%	6.847%
46	22.604	3298	3301	3309	rVB	196814	281732	5.32%	0.577%
47	23.174	3395	3398	3405	rVB	307134	454527	8.58%	0.931%
48	23.833	3506	3510	3515	rVB	362056	591476	11.16%	1.211%
49	23.910	3517	3523	3540	rVV3	1390176	3696583	69.78%	7.569%
50	24.080	3546	3552	3580	rVB	850723	3373662	63.68%	6.908%
51	24.586	3634	3638	3650	rVB	395067	811702	15.32%	1.662%

Sum of corrected areas: 48835454

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Instrument :
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ClientSampleId :
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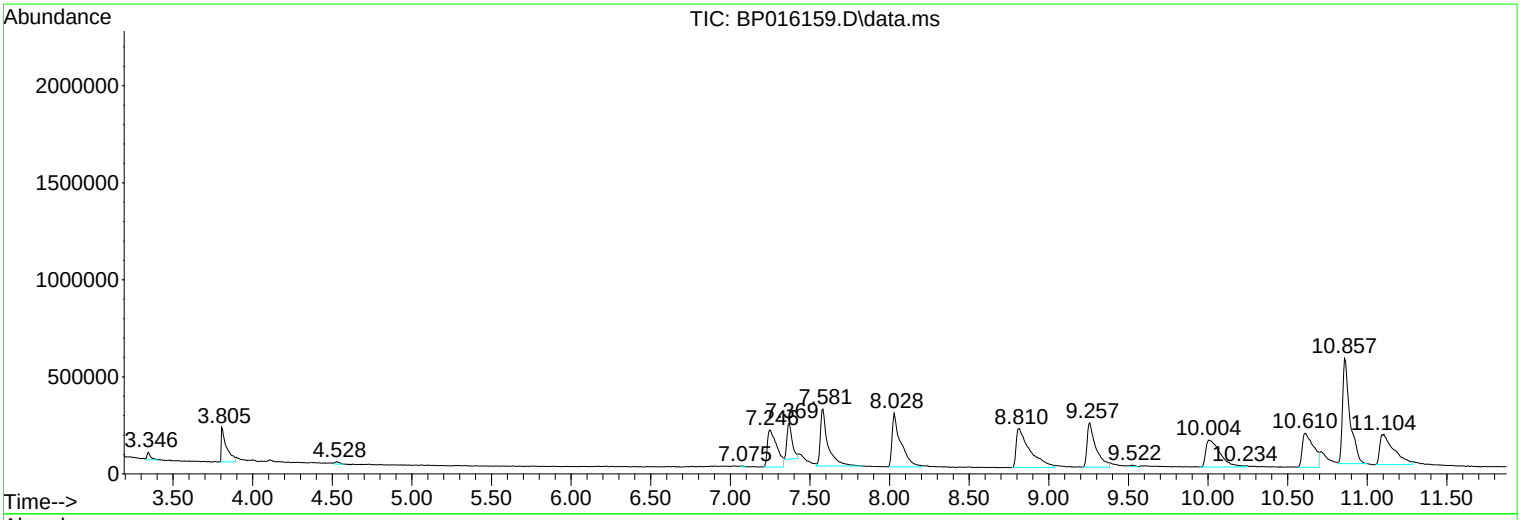
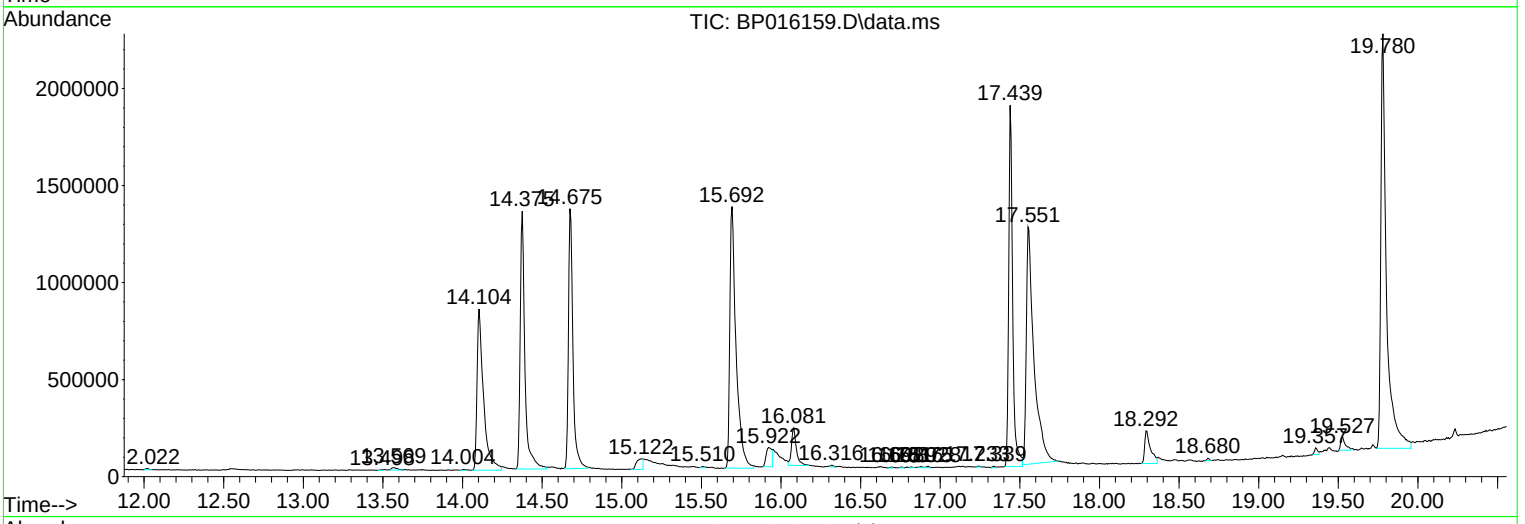
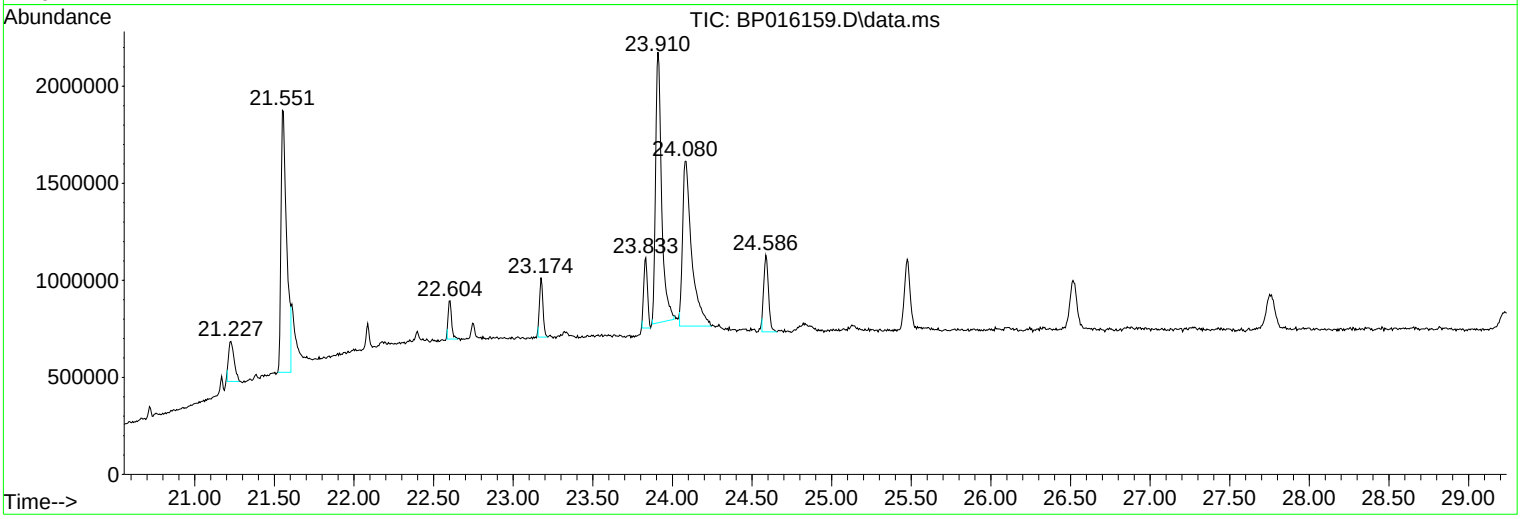
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016159.D
Acq On : 10 Jul 2023 15:16
Operator : MA/JU
Sample : 03404-03
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YBW41

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

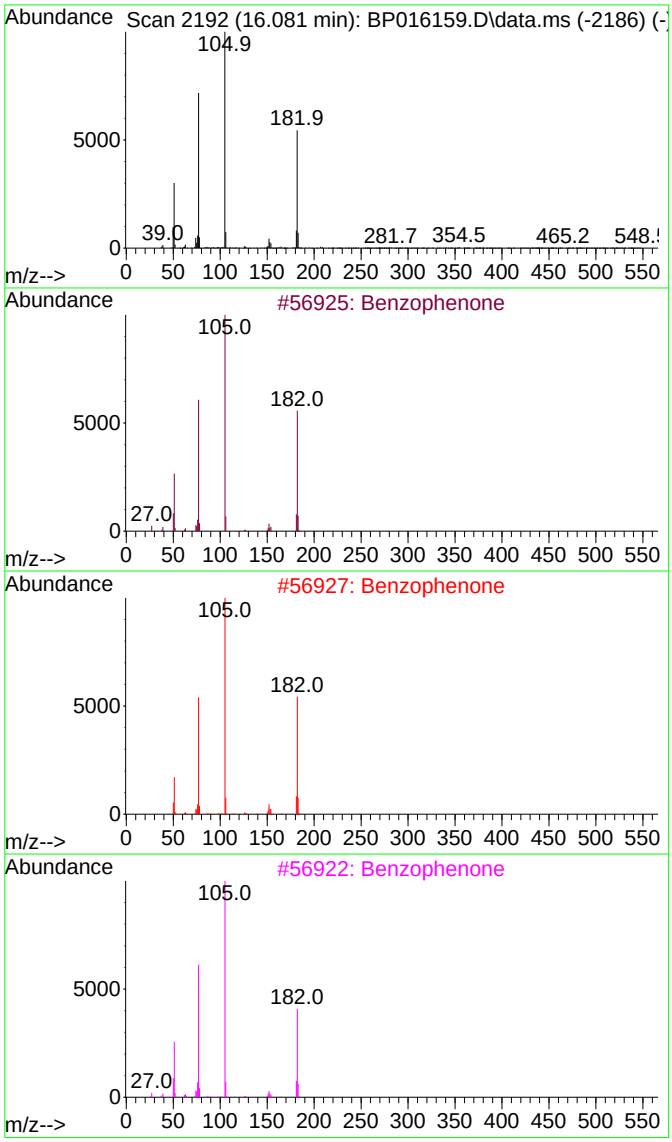
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

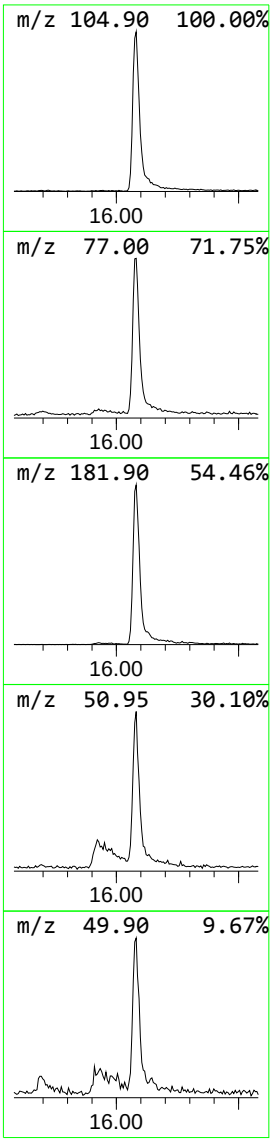
****

Peak Number 1 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.081	2.57 ng/ul	413522	Phenanthrene-d10	17.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	94
4	Benzophenone	182	C13H10O	000119-61-9	91
5	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016159.D
Acq On : 10 Jul 2023 15:16
Operator : MA/JU
Sample : 03404-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

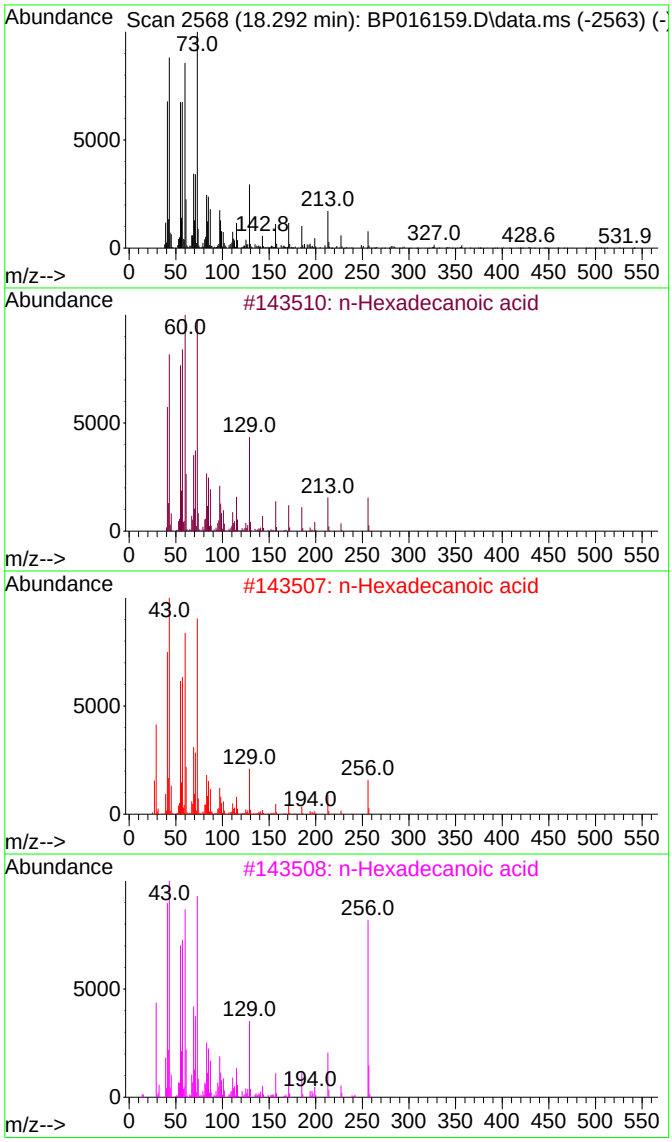
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

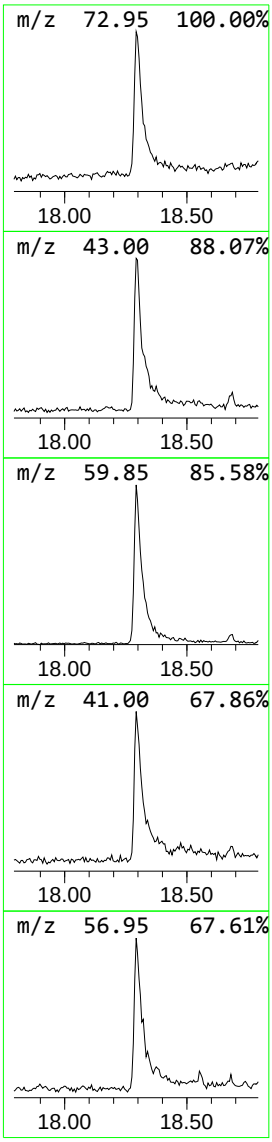
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.292	2.66 ng/ul	428424	Phenanthrene-d10	17.439

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	97
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5	Tridecanoic acid	214	C13H26O2	000638-53-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016159.D
Acq On : 10 Jul 2023 15:16
Operator : MA/JU
Sample : 03404-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YBW41

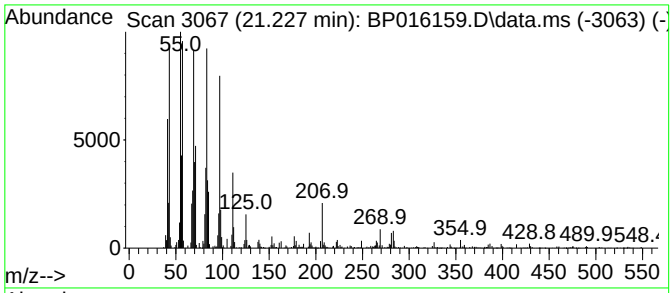
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

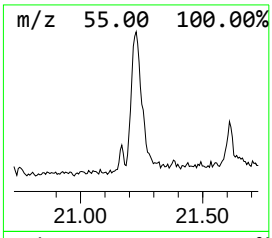
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

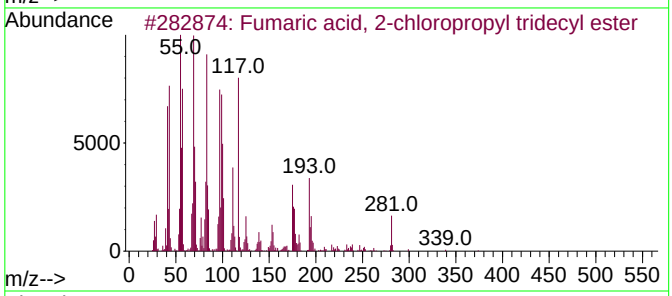
****
Peak Number 3 Fumaric acid, 2-chloropropy... Concentration Rank 3

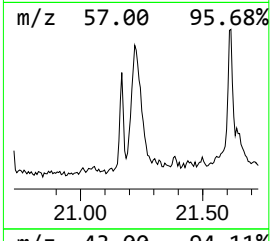
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	2.98 ng/ul	497702	Chrysene-d12	21.551

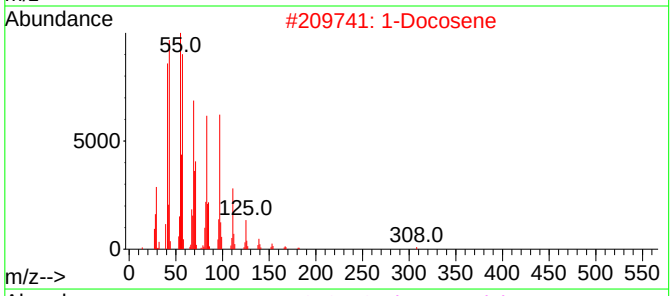
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1010348-57-1	97
2	1-Docosene	308	C22H44	001599-67-3	96
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94

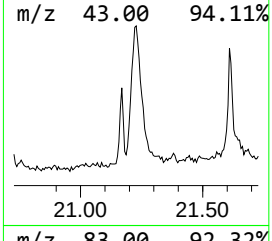


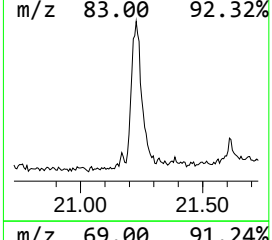


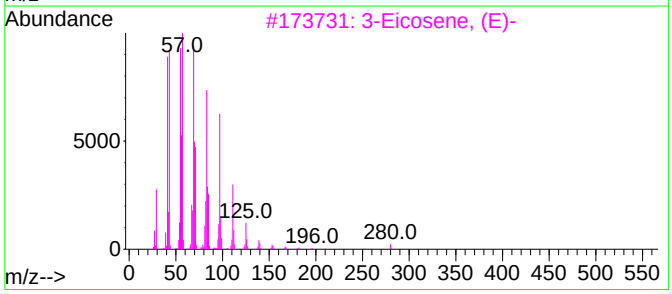


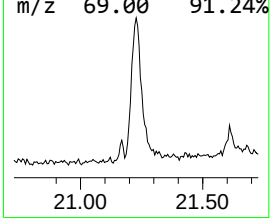












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016159.D
Acq On : 10 Jul 2023 15:16
Operator : MA/JU
Sample : 03404-03
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ALS Vial : 13 Sample Multiplier: 1

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BNA_P
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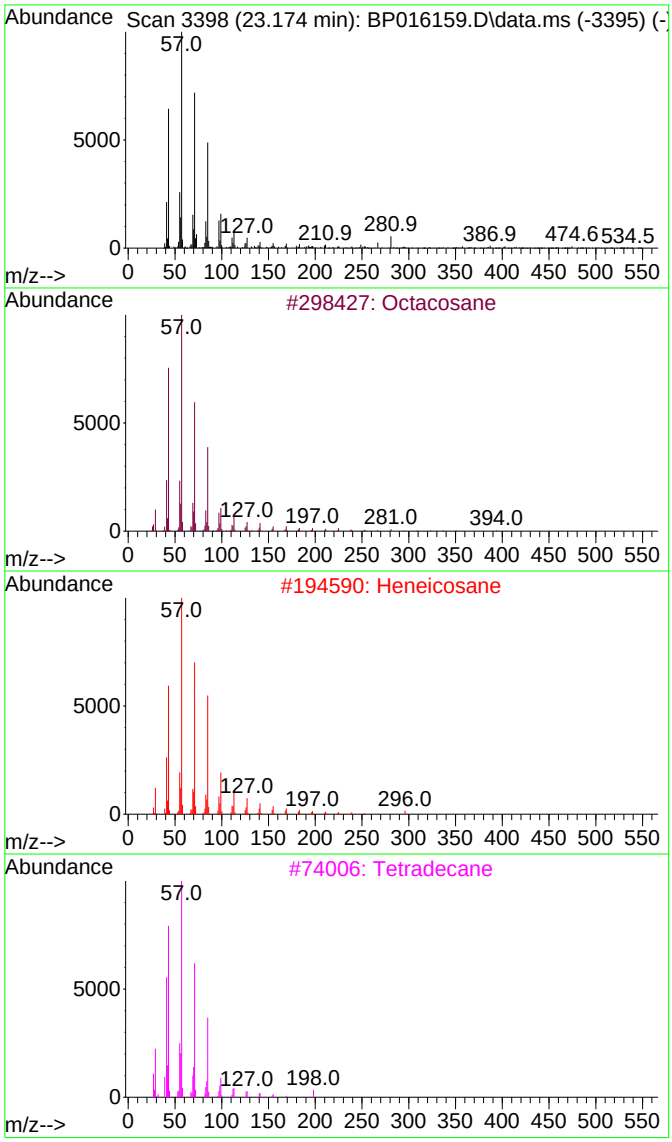
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

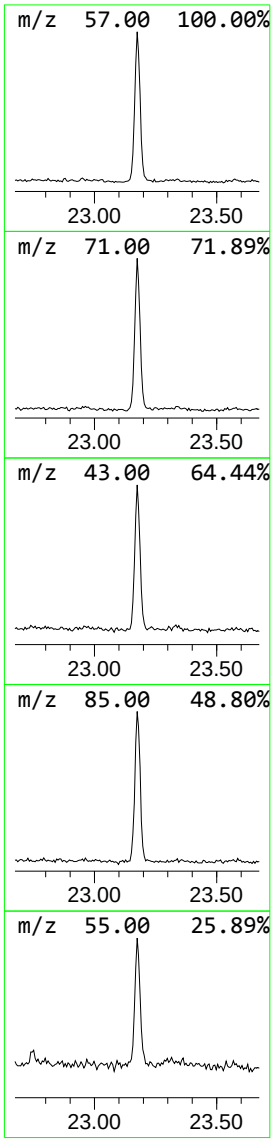
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.174	2.69 ng/ul	454527	Perylene-d12	24.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	83
2	Heneicosane	296	C21H44	000629-94-7	83
3	Tetradecane	198	C14H30	000629-59-4	74
4	Hexadecane	226	C16H34	000544-76-3	74
5	Tetracosane, 3-ethyl-	366	C26H54	055282-17-2	70





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Data File : BP016159.D
Acq On : 10 Jul 2023 15:16
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Sample : 03404-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YBW41

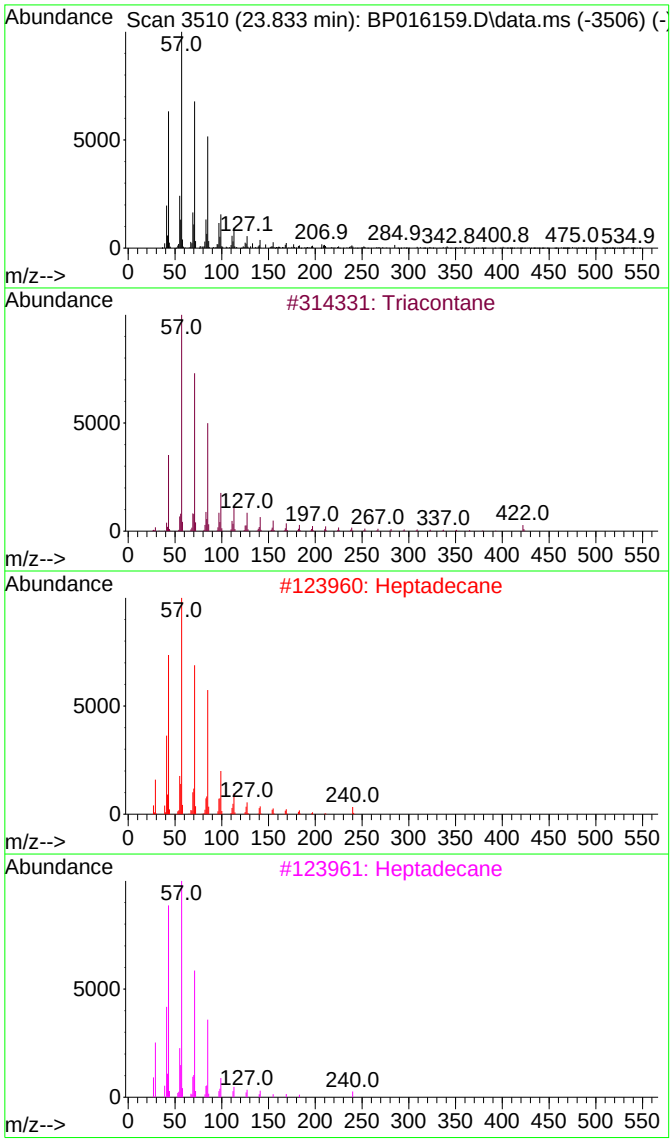
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

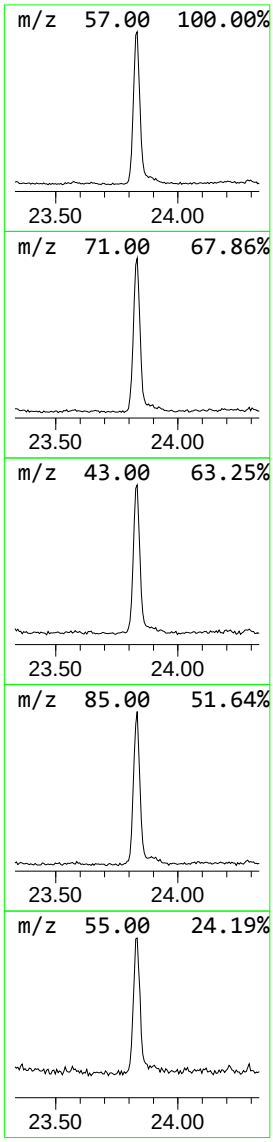
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.833	3.51 ng/ul	591476	Perylene-d12	24.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	97
2	Heptadecane	240	C17H36	000629-78-7	95
3	Heptadecane	240	C17H36	000629-78-7	95
4	Nonadecane	268	C19H40	000629-92-5	93
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016159.D
Acq On : 10 Jul 2023 15:16
Operator : MA/JU
Sample : 03404-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YBW41

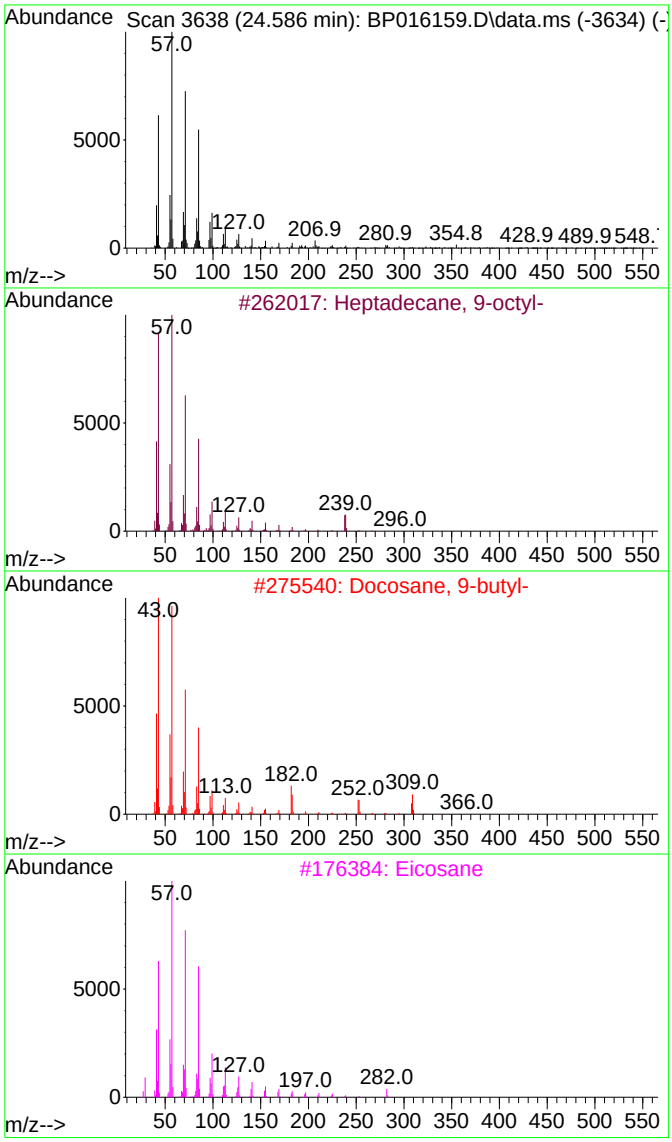
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

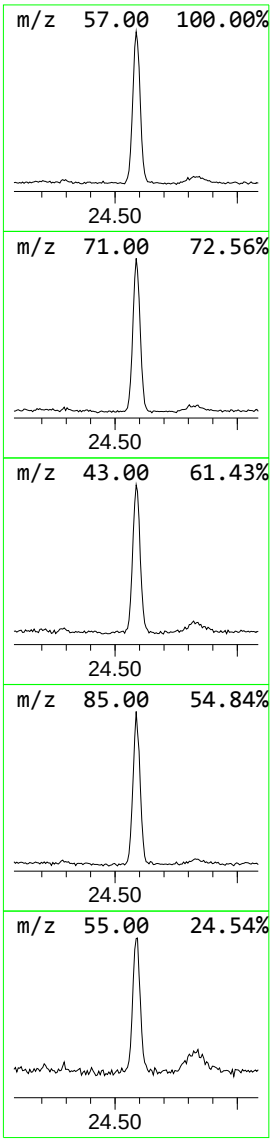
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.586	4.81 ng/ul	811702	Perylene-d12	24.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2	Docosane, 9-butyl-	366	C26H54	055282-14-9	93
3	Eicosane	282	C20H42	000112-95-8	93
4	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	93
5	Docosane, 5-butyl-	366	C26H54	055282-16-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071023\
Data File : BP016159.D
Acq On : 10 Jul 2023 15:16
Operator : MA/JU
Sample : 03404-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
YBW41

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzophenone	16.081	2.6	ng/ul	413522	4	17.439	3216930	20.0
n-Hexadecanoic ...	18.292	2.7	ng/ul	428424	4	17.439	3216930	20.0
Fumaric acid, 2...	21.227	3.0	ng/ul	497702	5	21.551	3343800	20.0
(DEL) Alkane: S...	23.174	2.7	ng/ul	454527	6	24.080	3373660	20.0
(DEL) Alkane: S...	23.833	3.5	ng/ul	591476	6	24.080	3373660	20.0
(DEL) Alkane: S...	24.586	4.8	ng/ul	811702	6	24.080	3373660	20.0