LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042023\
Data File : BM039530.D
Acq On : 20 Apr 2023 18:25
Operator : CG/JU
Sample : 02378-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : C0MK0

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-BM041823.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM039530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.213	26	30	39	rVB	55336	76166	1.04%	0.092%
2	3.525	81	83	94	rVB2	10837	21510	0.29%	0.026%
3	3.654	102	105	132	rVB	90964	225287	3.06%	0.272%
4	3.966	155	158	165	rVB	27200	34557	0.47%	0.042%
5	5.113	349	353	358	rVB	24780	31005	0.42%	0.037%
6	5.460	406	412	419	rBV6	14792	45848	0.62%	0.055%
7	7.013	670	676	692	rVV	137529	333215	4.53%	0.402%
8	7.154	694	700	724	rVV	717840	1260538	17.14%	1.521%
9	7.354	728	734	760	rVB	699314	1281761	17.43%	1.547%
10	7.707	789	794	806	rBV	131200	213318	2.90%	0.257%
11	7.819	806	813	817	rBV	779494	1313632	17.86%	1.585%
12	7.854	817	819	833	rVB	366792	590598	8.03%	0.713%
13	8.178	868	874	886	rVB	89374	165148	2.25%	0.199%
14	8.484	921	926	928	rBV6	5163	7583	0.10%	0.009%
15	8.554	931	938	957	rBV	519692	1078204	14.66%	1.301%
16	8.713	960	965	972	rVB	15706	38474	0.52%	0.046%
17	8.995	1006	1013	1034	rBV	875622	1564576	21.27%	1.888%
18	9.384	1075	1079	1084	rVB	13902	22333	0.30%	0.027%
19	9.719	1129	1136	1152	rVV	726923	1336067	18.17%	1.612%
20	10.054	1184	1193	1195	rBV8	4866	9973	0.14%	0.012%
21	10.266	1222	1229	1249	rBV	852151	1947819	26.49%	2.351%
22	10.495	1264	1268	1275	rVB3	19191	32479	0.44%	0.039%
23	10.631	1284	1291	1310	rBV	1163544	2046834	27.83%	2.470%
24	10.795	1310	1319	1344	rBV	402761	1069959	14.55%	1.291%
25	11.066	1364	1365	1372	rVB7	6615	8937	0.12%	0.011%
26	11.877	1500	1503	1514	rVB5	9031	18848	0.26%	0.023%
27	11.972	1514	1519	1522	rBV6	5933	11436	0.16%	0.014%
28	12.054	1529	1533	1543	rVB6	7446	14377	0.20%	0.017%
29	12.230	1558	1563	1570	rVB	14907	25301	0.34%	0.031%
30	12.683	1633	1640	1642	rBV6	7622	12609	0.17%	0.015%
31	13.295	1739	1744	1747	rBV5	15208	28879	0.39%	0.035%
32	13.372	1755	1757	1763	rVB5	7122	10791	0.15%	0.013%
33	13.460	1768	1772	1776	rBV6	5483	9412	0.13%	0.011%
34	13.560	1781	1789	1795	rBV3	12277	28963	0.39%	0.035%
35	13.795	1821	1829	1834	rBV9	12476	24106	0.33%	0.029%
36	13.895	1837	1846	1860	rBV	2427822	3486285	47.41%	4.207%

LSC Area Percent Report

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Misc :
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Instrument :
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ClientSampleId :
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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
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Title : SVOA CALIBRATION

37	14.001	1860	1864	1869	rVB7	13933	25172	0.34%	0.030%
38	14.083	1873	1878	1883	rBV	22994	35111	0.48%	0.042%
39	14.171	1883	1893	1906	rBV	2471018	3837613	52.18%	4.631%
40	14.301	1911	1915	1921	rVB3	30200	53965	0.73%	0.065%
41	14.371	1923	1927	1931	rVB4	7782	10554	0.14%	0.013%
42	14.477	1939	1945	1959	rBV	1853828	2807326	38.17%	3.388%
43	14.624	1967	1970	1975	rVB6	12307	18210	0.25%	0.022%
44	14.736	1982	1989	1997	rBV5	60002	199696	2.72%	0.241%
45	14.907	2013	2018	2020	rBV6	12377	21043	0.29%	0.025%
46	14.936	2021	2023	2030	rVB6	19665	25537	0.35%	0.031%
47	15.189	2037	2066	2067	rBV	163883	1204497	16.38%	1.454%
48	15.477	2109	2115	2132	rVB	3249848	4816364	65.49%	5.813%
49	15.607	2132	2137	2152	rVB	995912	1511979	20.56%	1.825%
50	15.842	2172	2177	2190	rVB	2074426	2883339	39.21%	3.480%
51	16.407	2269	2273	2280	rVB	176108	238540	3.24%	0.288%
52	16.636	2308	2312	2323	rBV	167582	288385	3.92%	0.348%
53	17.230	2407	2413	2423	rBV	2089018	3069664	41.74%	3.705%
54	17.330	2424	2430	2440	rVV2	3321258	4886188	66.44%	5.897%
55	18.142	2562	2568	2583	rBV	4332994	6678929	90.82%	8.060%
56	19.418	2780	2785	2806	rVB	4417712	5937621	80.74%	7.166%
57	19.630	2816	2821	2839	rVB	3604378	5023982	68.31%	6.063%
58	20.165	2910	2912	2921	rVB2	81937	97962	1.33%	0.118%
59	20.736	3006	3009	3014	rVB4	78183	91052	1.24%	0.110%
60	20.953	3044	3046	3051	rBV3	56090	63076	0.86%	0.076%
61	21.059	3061	3064	3071	rVB2	349200	535362	7.28%	0.646%
62	21.136	3073	3077	3088	rVB	513385	932920	12.69%	1.126%
63	21.277	3097	3101	3106	rBV3	219478	341176	4.64%	0.412%
64	21.424	3121	3126	3139	rBV	1766217	2526608	34.36%	3.049%
65	22.024	3224	3228	3231	rBV	174457	214907	2.92%	0.259%
66	23.047	3398	3402	3411	rBV	291026	517833	7.04%	0.625%
67	23.636	3495	3502	3516	rBV2	2100608	4414135	60.02%	5.327%
68	23.788	3522	3528	3542	rVB2	1120370	2300177	31.28%	2.776%
69	24.883	3709	3714	3737	rVB5	391454	1470892	20.00%	1.775%
70	25.183	3756	3765	3780	rBV7	1681262	7354152	100.00%	8.875%

Sum of corrected areas: 82860795

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Instrument :
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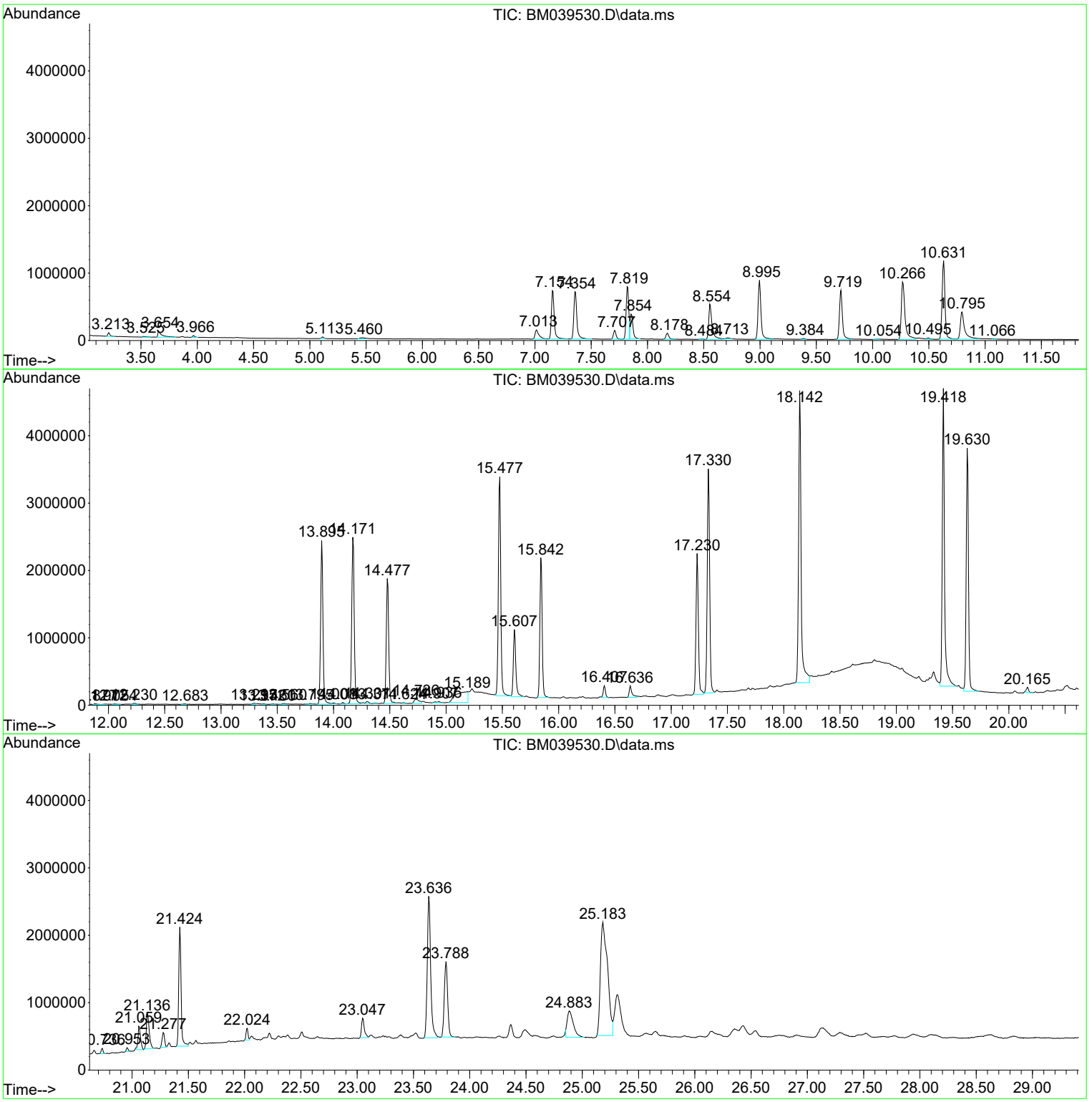
ClientSampleId :
C0MK0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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



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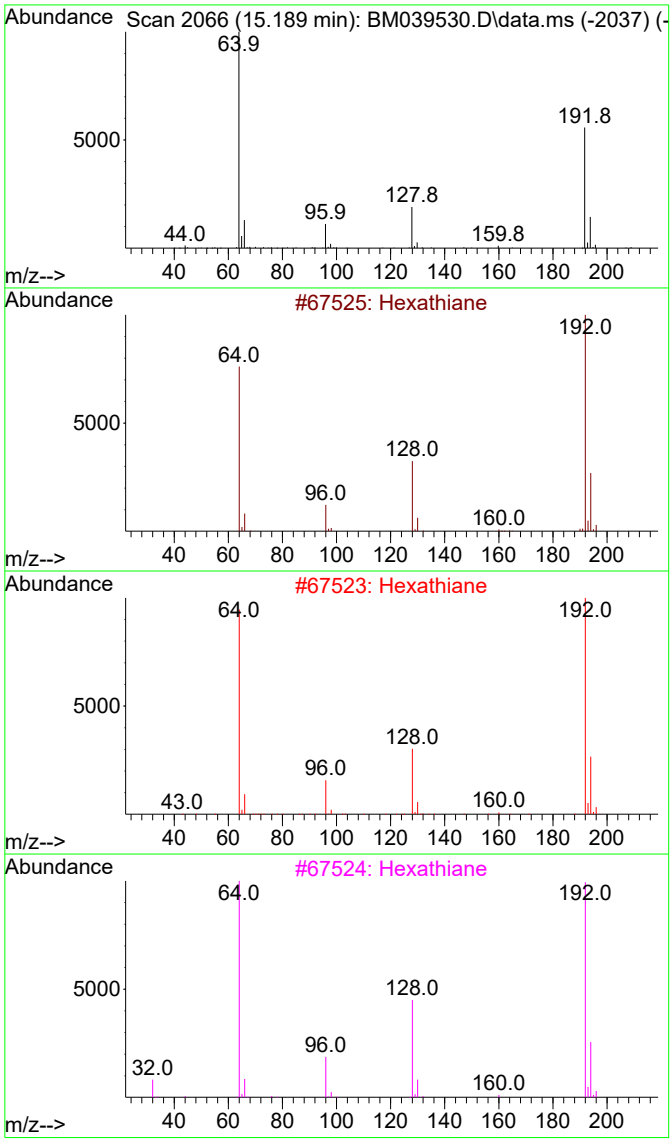
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

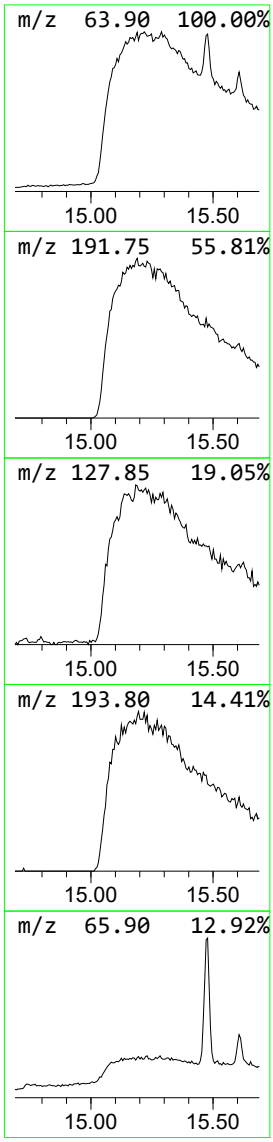
****

Peak Number 3 Hexathiane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.189	8.58 ng/ul	1204500	Acenaphthene-d10	14.477

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexathiane	192	S6	013798-23-7	91
2	Hexathiane	192	S6	013798-23-7	91
3	Hexathiane	192	S6	013798-23-7	91
4	Di(tert-butyl) trisulfide, perfl...	534	C8F18S3	016005-64-4	9
5	dimethyl tellurenyl	192	C2H6STe	1000374-19-6	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042023\
Data File : BM039530.D
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Sample : 02378-07
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

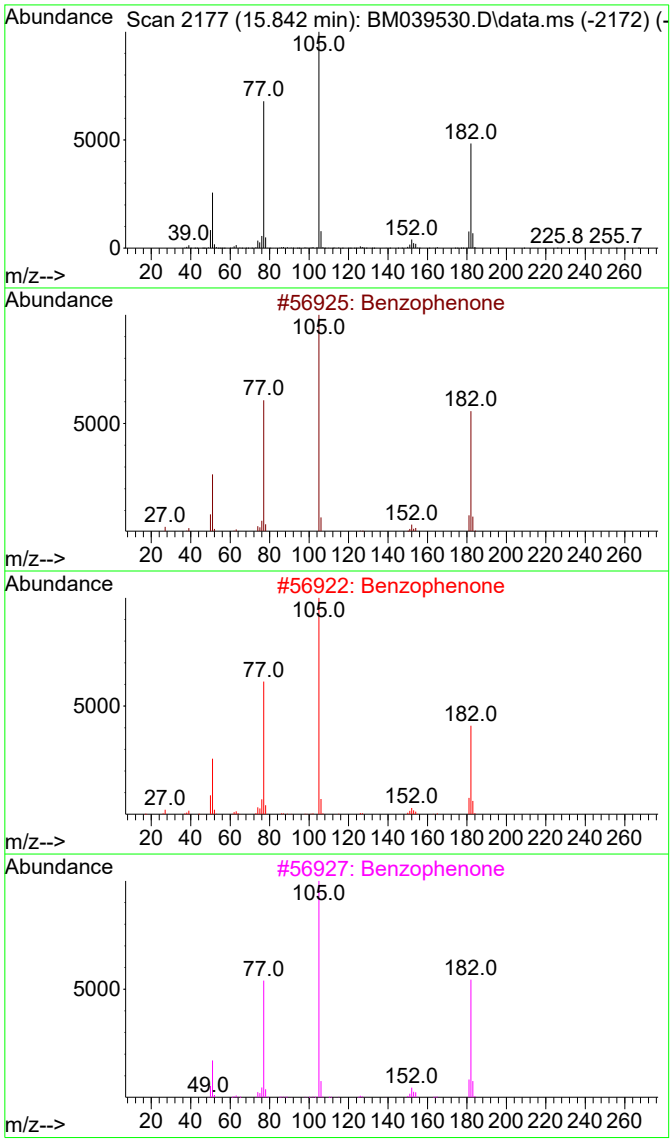
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

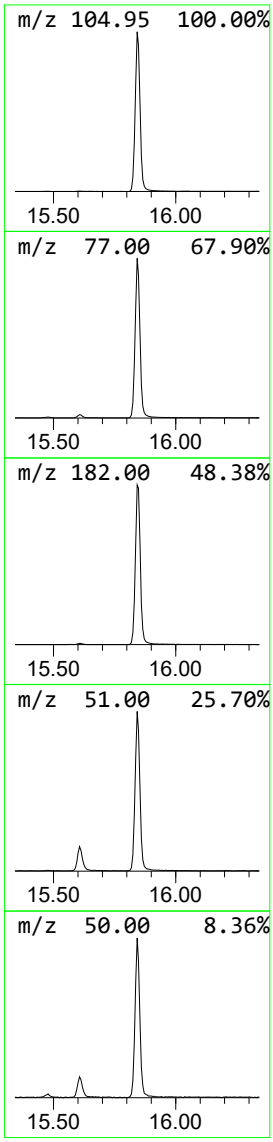
****

Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.842	20.54 ng/ul	2883340	Acenaphthene-d10	14.477

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	96
3	Benzophenone	182	C13H10O	000119-61-9	95
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	91





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Data File : BM039530.D
Acq On : 20 Apr 2023 18:25
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Sample : 02378-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK0

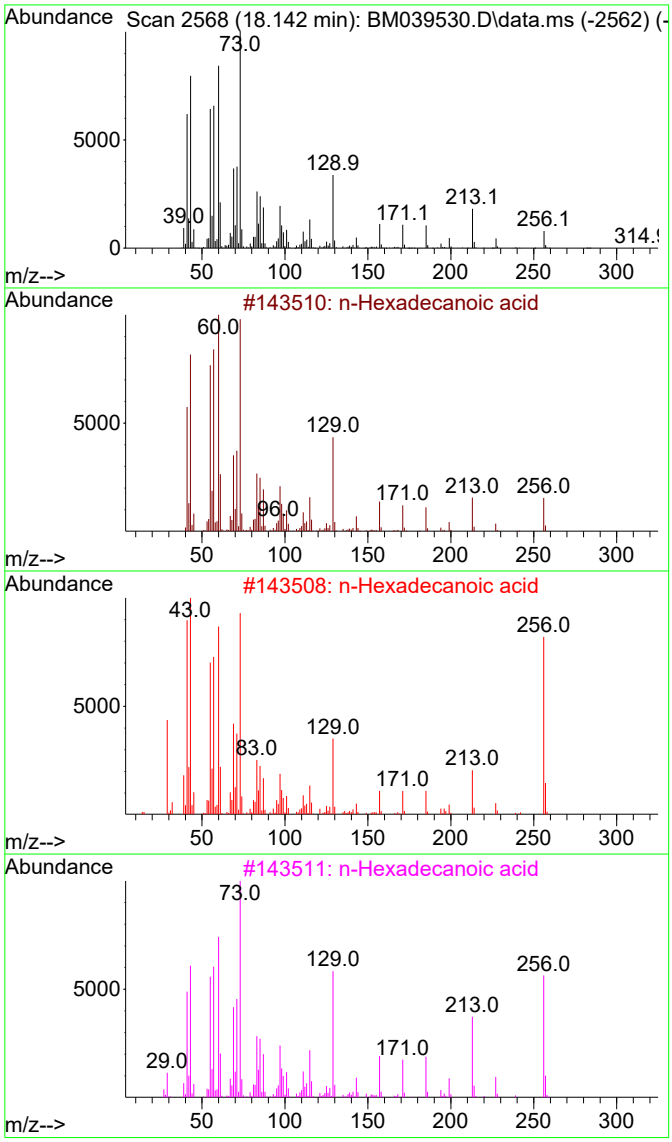
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

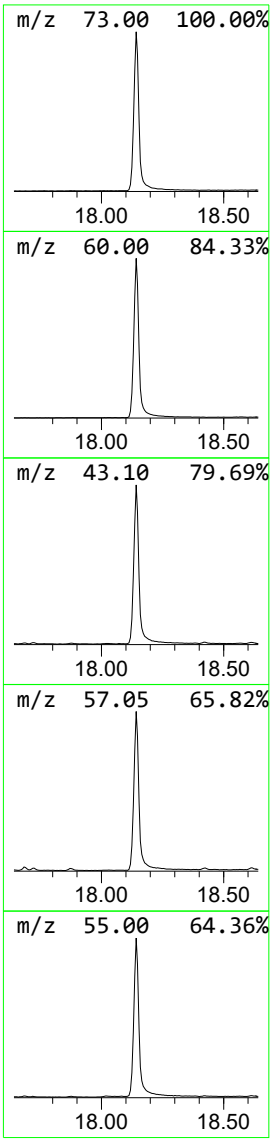
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.142	43.52 ng/ul	6678930	Phenanthrene-d10	17.230

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	98
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	94





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

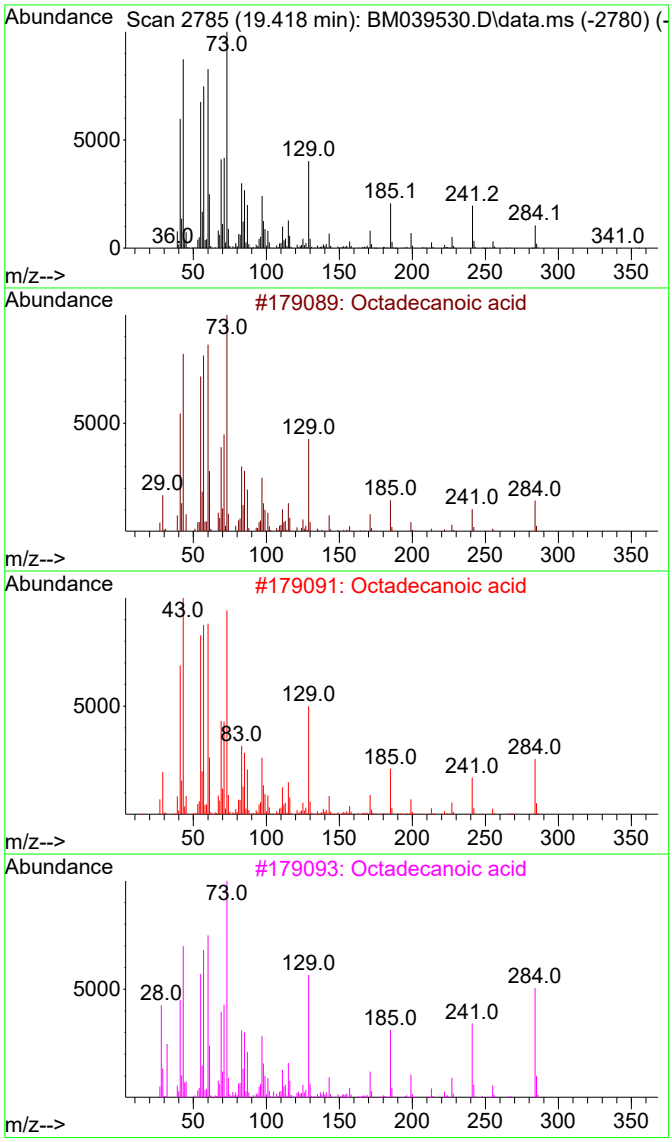
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

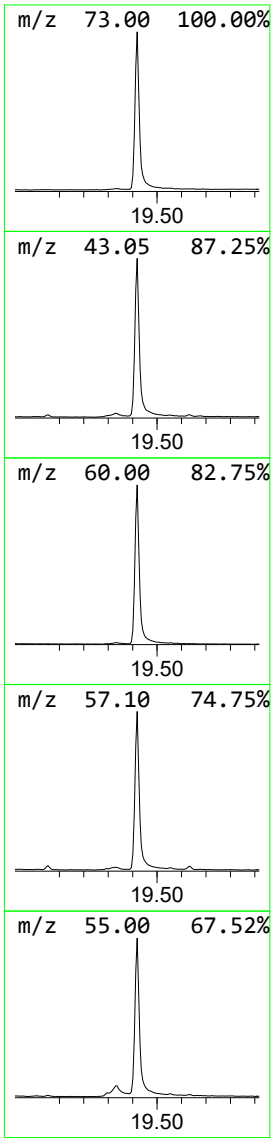
****

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.418	47.00 ng/ul	5937620	Chrysene-d12	21.424

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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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK0

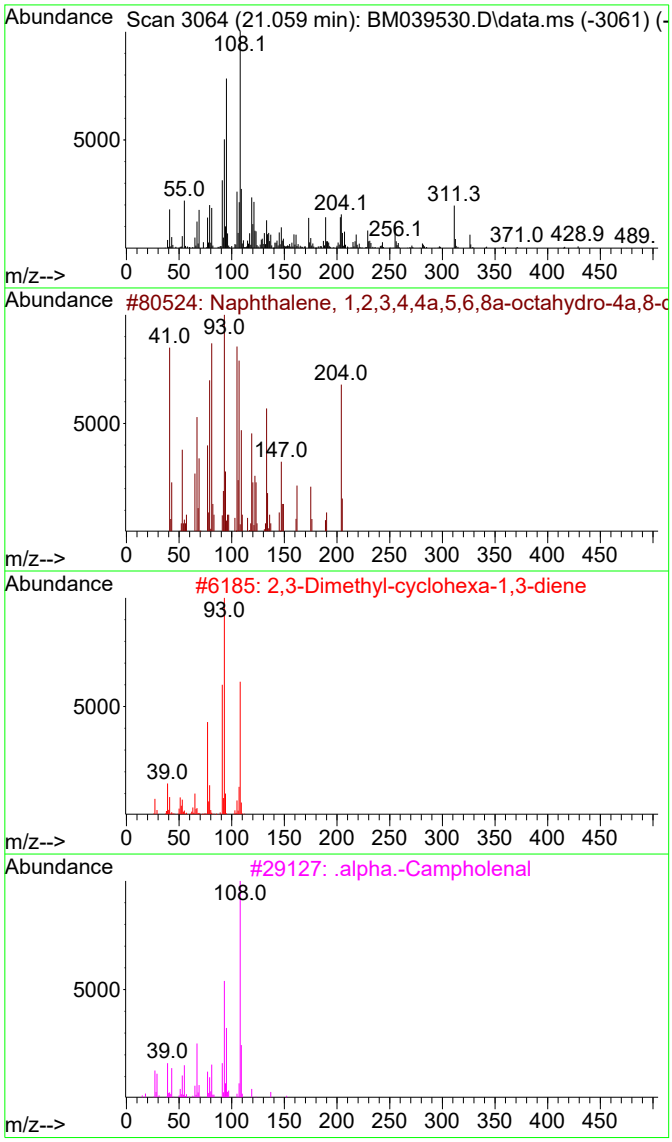
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

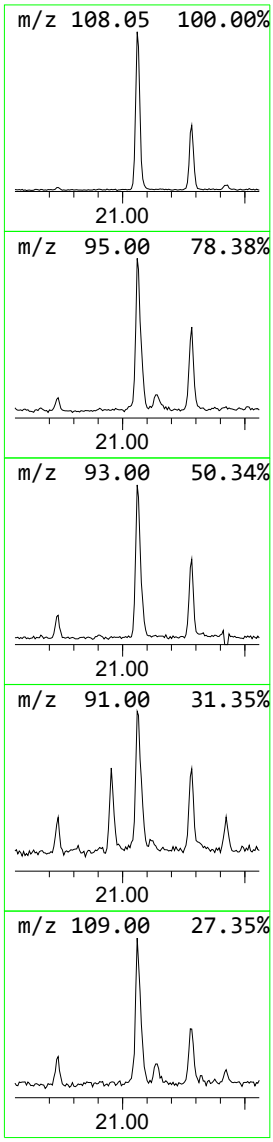
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1,2,3,4,4a,5,6... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.059	4.24 ng/ul	535362	Chrysene-d12	21.424

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	56
2	2,3-Dimethyl-cyclohexa-1,3-diene	108	C8H12	004430-91-5	43
3	.alpha.-Campholenal	152	C10H16O	004501-58-0	43
4	1,4-DIMETHYL-CYCLOHEXA-1,3-DIENE	108	C8H12	026120-52-5	38
5	Santolina epoxide	152	C10H16O	060485-45-2	38





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BNA_M
ClientSampleId :
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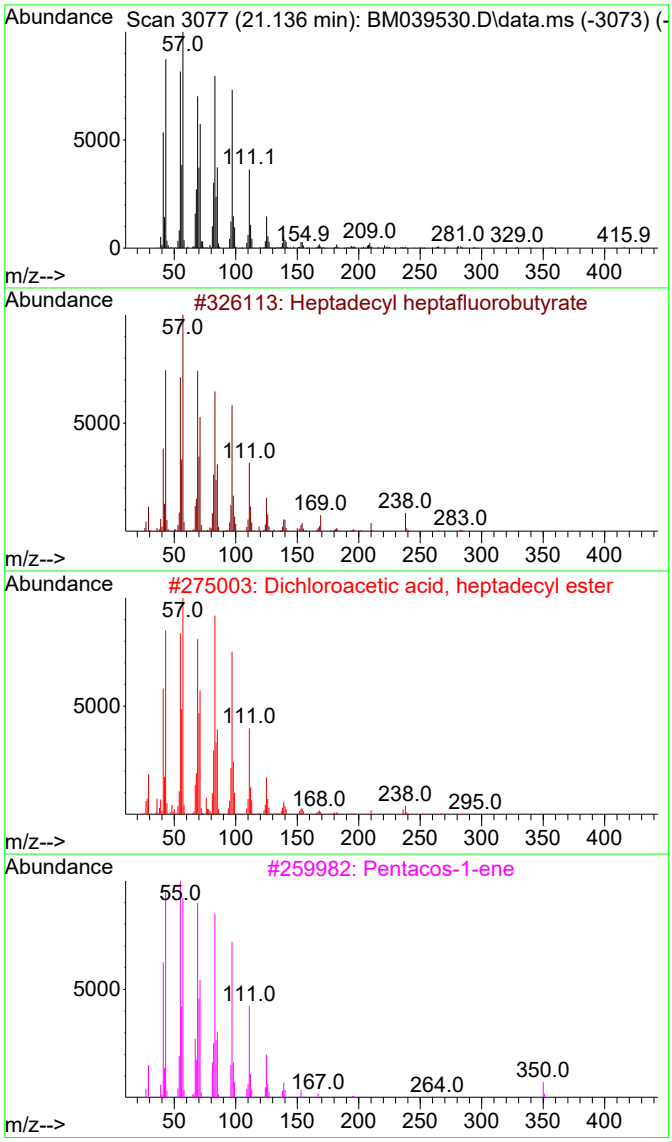
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

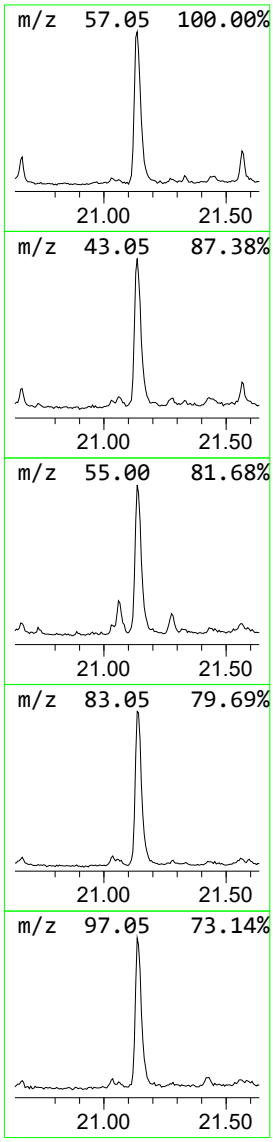
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.136	7.38 ng/ul	932920	Chrysene-d12	21.424

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
3	Pentacos-1-ene	350	C25H50	016980-85-1	91
4	1-Tricosene	322	C23H46	018835-32-0	91
5	Nonacos-1-ene	406	C29H58	018835-35-3	91





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Data File : BM039530.D
Acq On : 20 Apr 2023 18:25
Operator : CG/JU
Sample : 02378-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

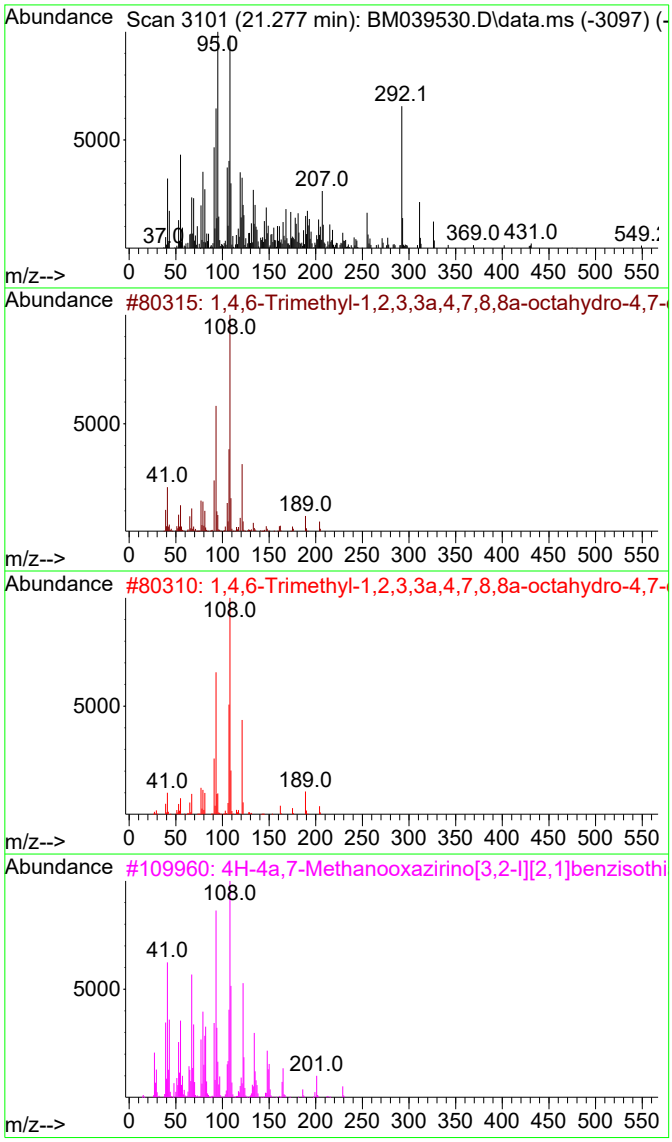
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

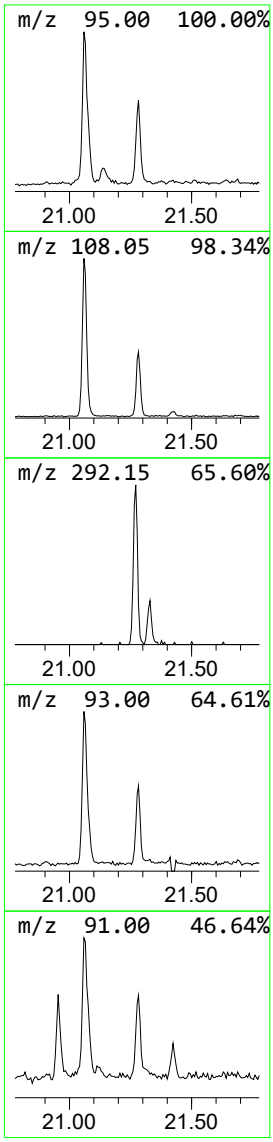
****

Peak Number 9 unknown-01 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.277	2.70 ng/ul	341176	Chrysene-d12	21.424

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,6-Trimethyl-1,2,3,3a,4,7,8,8...	204	C15H24	065128-08-7	42
2	1,4,6-Trimethyl-1,2,3,3a,4,7,8,8...	204	C15H24	065128-08-7	38
3	4H-4a,7-Methanooxazirino[3,2-I][...	229	C10H15NO3S	104322-63-6	25
4	Allophanic acid, 4-benzoyl-, m-t...	298	C16H14N2O4	1000160-28-4	25
5	1H-Pyrazole, 1-methyl-3-vinyl-	108	C6H8N2	056342-53-1	22





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Acq On : 20 Apr 2023 18:25
Operator : CG/JU
Sample : 02378-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK0

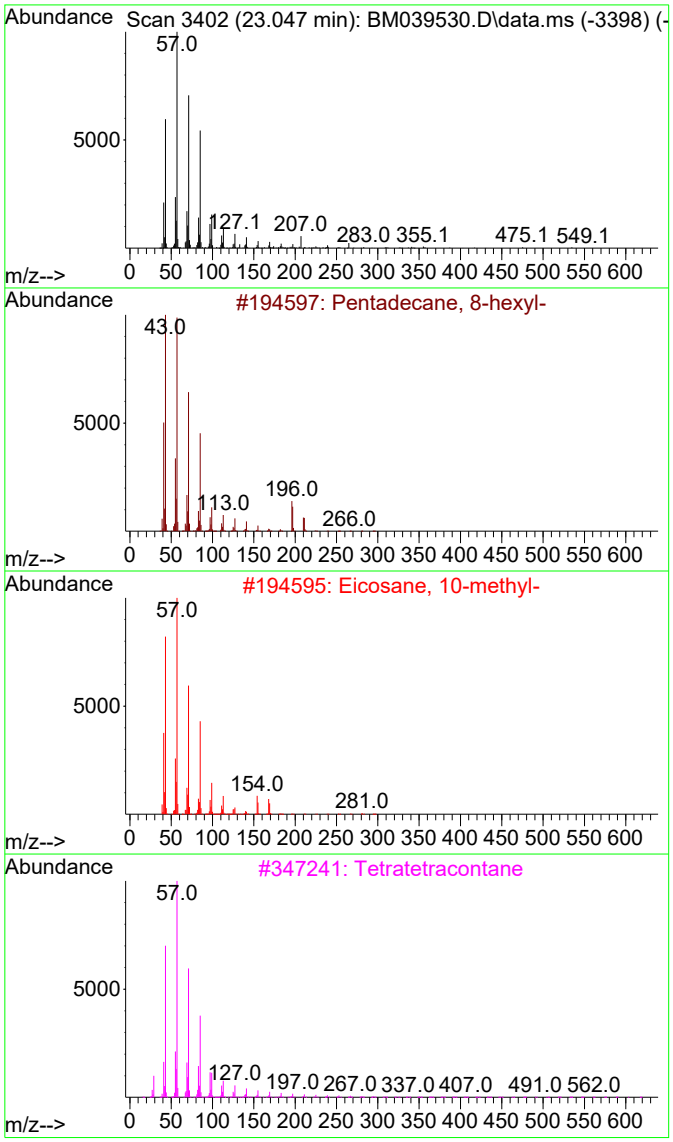
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

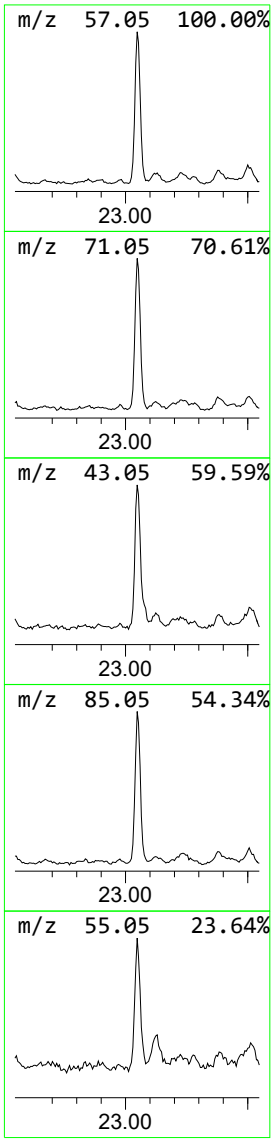
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.047	4.50 ng/ul	517833	Perylene-d12	23.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Octacosane	394	C28H58	000630-02-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042023\
Data File : BM039530.D
Acq On : 20 Apr 2023 18:25
Operator : CG/JU
Sample : 02378-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK0

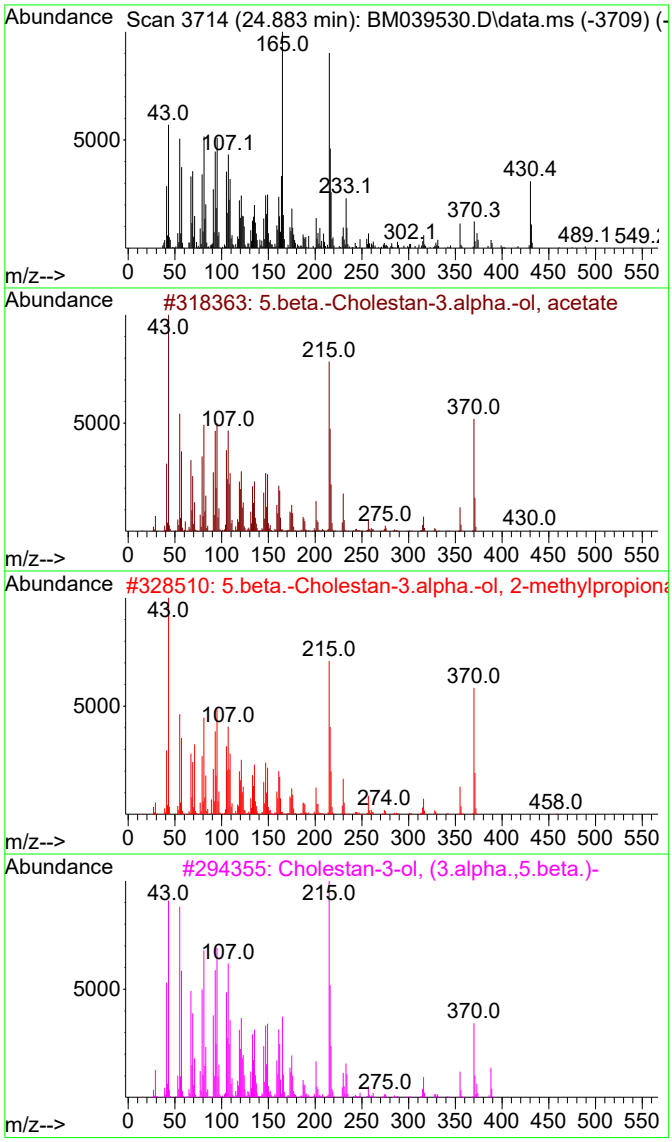
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

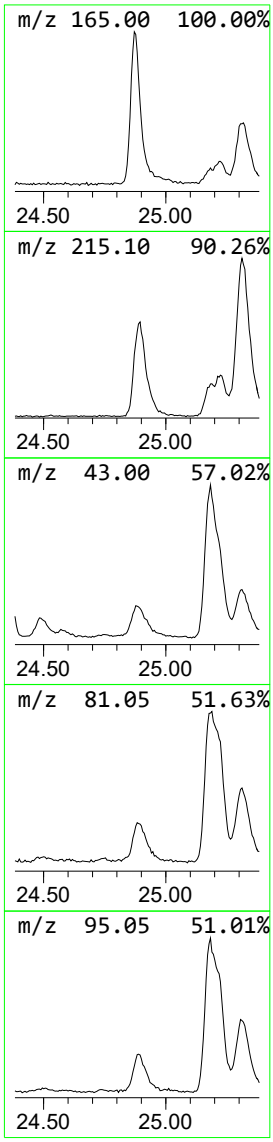
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 5.beta.-Cholestan-3.alpha.-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.883	12.79 ng/ul	1470890	Perylene-d12	23.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5.beta.-Cholestan-3.alpha.-ol, a...	430	C29H50O2	033157-47-0	53
2	5.beta.-Cholestan-3.alpha.-ol, 2...	458	C31H54O2	1000514-95-7	46
3	Cholestan-3-ol, (3.alpha.,5.beta.)-	388	C27H48O	000516-92-7	38
4	Cholestan-3-ol, (3.alpha.,5.beta.)-	388	C27H48O	000516-92-7	38
5	Vitamin E	430	C29H50O2	000059-02-9	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042023\
Data File : BM039530.D
Acq On : 20 Apr 2023 18:25
Operator : CG/JU
Sample : 02378-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

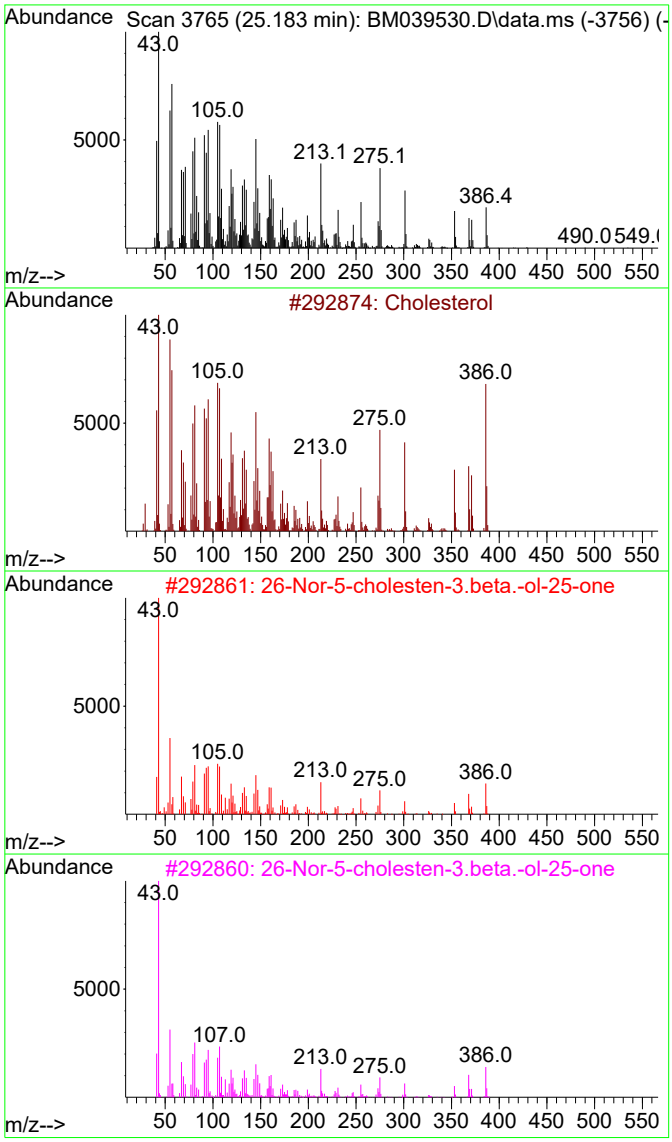
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

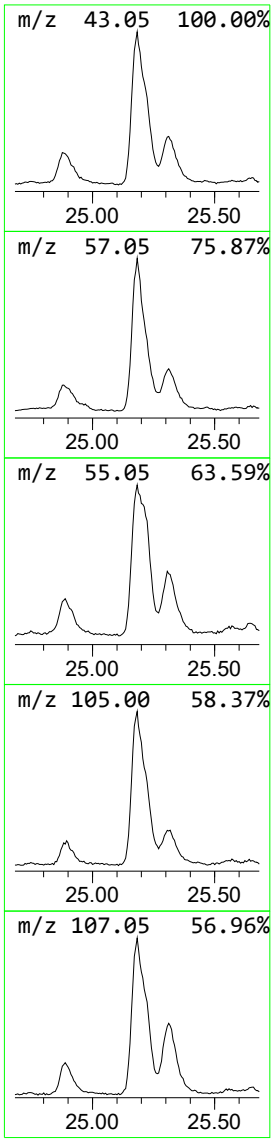
****

Peak Number 12 Cholesterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.183	63.94 ng/ul	7354150	Perylene-d12	23.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	93
4	Lathosterol	386	C27H46O	000080-99-9	90
5	Cholesterol	386	C27H46O	000057-88-5	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042023\
Data File : BM039530.D
Acq On : 20 Apr 2023 18:25
Operator : CG/JU
Sample : 02378-07
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0MK0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.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
Hexathiane	15.189	8.6	ng/ul	1204500	3	14.477	2807330	20.0
Benzophenone	15.842	20.5	ng/ul	2883340	3	14.477	2807330	20.0
n-Hexadecanoic ...	18.142	43.5	ng/ul	6678930	4	17.230	3069660	20.0
Octadecanoic acid	19.418	47.0	ng/ul	5937620	5	21.424	2526610	20.0
Naphthalene, 1,...	21.059	4.2	ng/ul	535362	5	21.424	2526610	20.0
Heptadecyl hept...	21.136	7.4	ng/ul	932920	5	21.424	2526610	20.0
unknown-01	21.277	2.7	ng/ul	341176	5	21.424	2526610	20.0
(DEL) Alkane: S...	23.047	4.5	ng/ul	517833	6	23.788	2300180	20.0
5.beta.-Cholest...	24.883	12.8	ng/ul	1470890	6	23.788	2300180	20.0
Cholesterol	25.183	63.9	ng/ul	7354150	6	23.788	2300180	20.0