LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DCGM8

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_G\Methods\SFAM-EPA-BG070123.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG057982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.118	3	5	28	rVB	1706973	2038481	23.57%	7.738%
2	3.376	45	49	58	rVB2	8907	14706	0.17%	0.056%
3	3.788	114	119	130	rBV	82873	135368	1.57%	0.514%
4	3.899	133	138	145	rVB5	6102	10510	0.12%	0.040%
5	4.023	155	159	165	rVB	13912	22595	0.26%	0.086%
6	4.346	209	214	221	rVB	11546	16596	0.19%	0.063%
7	7.107	677	684	693	rBV	129077	220371	2.55%	0.836%
8	7.266	704	711	720	rBV	114013	187719	2.17%	0.713%
9	7.472	739	746	756	rVB	133117	224969	2.60%	0.854%
10	7.942	819	826	833	rBV	148379	242481	2.80%	0.920%
11	8.647	938	946	954	rBV2	97426	171452	1.98%	0.651%
12	9.099	1017	1023	1031	rBV	133688	241317	2.79%	0.916%
13	9.822	1138	1146	1154	rBV	108968	193103	2.23%	0.733%
14	10.362	1231	1238	1249	rBV	157441	284101	3.28%	1.078%
15	10.744	1293	1303	1313	rBV	225301	396719	4.59%	1.506%
16	10.879	1318	1326	1334	rBV	85951	158633	1.83%	0.602%
17	13.459	1761	1765	1769	rBV3	8027	11727	0.14%	0.045%
18	13.976	1846	1853	1859	rBV	317953	455424	5.27%	1.729%
19	14.270	1897	1903	1912	rVB	369766	583805	6.75%	2.216%
20	14.575	1948	1955	1962	rBV	349741	544506	6.30%	2.067%
21	14.775	1982	1989	2001	rBV	116293	206596	2.39%	0.784%
22	15.562	2115	2123	2135	rBV	485178	740660	8.56%	2.811%
23	15.680	2137	2143	2152	rBV	98268	149275	1.73%	0.567%
24	15.921	2180	2184	2191	rVB	50415	71091	0.82%	0.270%
25	16.702	2314	2317	2321	rBV3	10455	15187	0.18%	0.058%
26	17.066	2374	2379	2383	rBV3	19838	25530	0.30%	0.097%
27	17.266	2409	2413	2416	rVV5	8643	12139	0.14%	0.046%
28	17.319	2416	2422	2428	rVV	440461	649123	7.50%	2.464%
29	17.413	2432	2438	2445	rVB	407443	613192	7.09%	2.328%
30	17.977	2531	2534	2537	rVB3	9107	10796	0.12%	0.041%
31	18.077	2547	2551	2556	rBV4	12613	19624	0.23%	0.074%
32	18.141	2557	2562	2567	rBV	121038	169237	1.96%	0.642%
33	18.200	2567	2572	2583	rVV	365681	524582	6.07%	1.991%
34	18.494	2619	2622	2625	rBV4	14686	17324	0.20%	0.066%
35	18.541	2626	2630	2637	rVV3	32325	54910	0.63%	0.208%
36	18.700	2653	2657	2662	rBV7	8377	15216	0.18%	0.058%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

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_G\Methods\SFAM-EPA-BG070123.MA.M
Title : SVOA CALIBRATION

37	19.328	2761	2764	2765	rBV2	22932	22608	0.26%	0.086%
38	19.475	2784	2789	2796	rBV	74391	108607	1.26%	0.412%
39	19.704	2822	2828	2836	rBV	607563	911680	10.54%	3.460%
40	19.851	2850	2853	2857	rBV	38083	52975	0.61%	0.201%
41	21.214	3081	3085	3093	rBV	163609	344980	3.99%	1.309%
42	21.573	3140	3146	3153	rBV	389652	620894	7.18%	2.357%
43	23.817	3523	3528	3534	rVB	175569	341710	3.95%	1.297%
44	24.516	3640	3647	3659	rVB2	296028	814311	9.41%	3.091%
45	24.740	3678	3685	3696	rVB2	262730	768022	8.88%	2.915%
46	25.856	3868	3875	3887	rVB3	270591	834760	9.65%	3.169%
47	28.805	4369	4377	4395	rVB4	216299	939517	10.86%	3.566%
48	31.479	4811	4832	4854	rVB3	1447826	8649300	100.00%	32.830%
49	32.207	4943	4956	4978	rVB8	440723	2486928	28.75%	9.440%

Sum of corrected areas: 26345357

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ALS Vial : 39 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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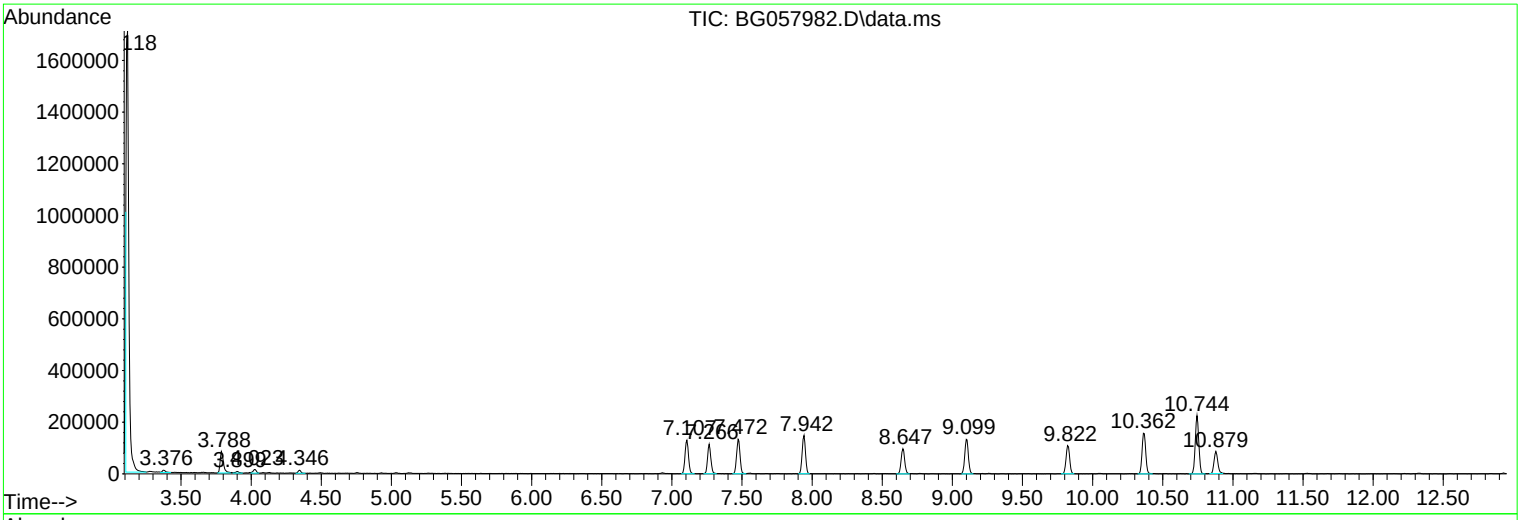
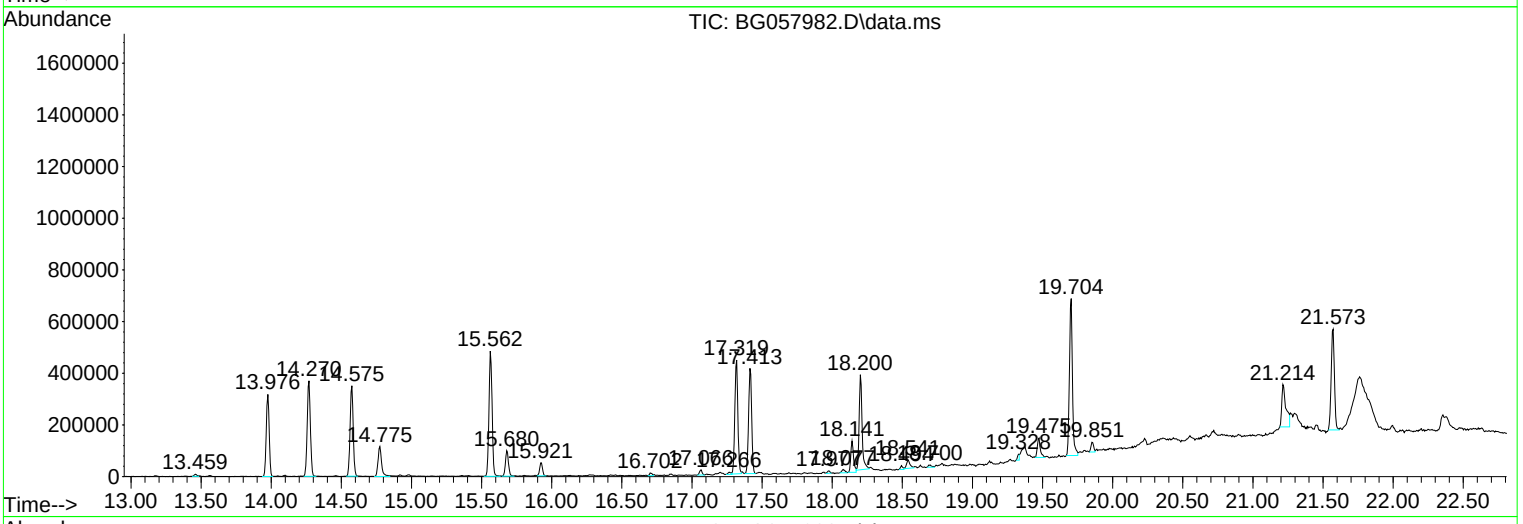
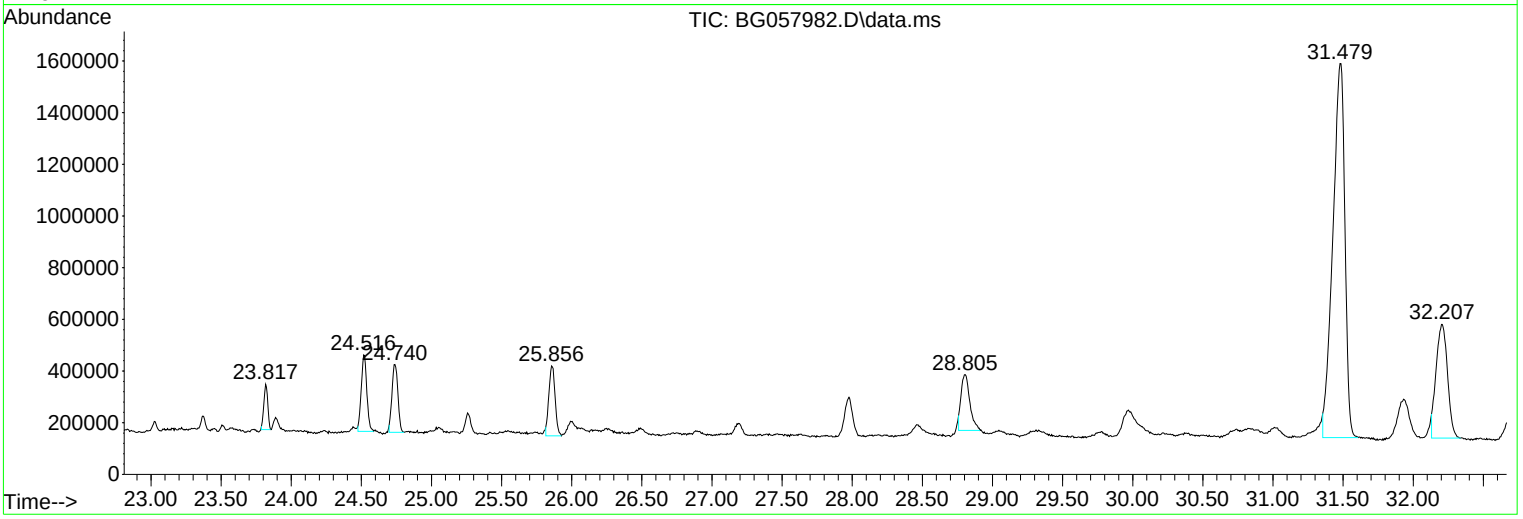
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

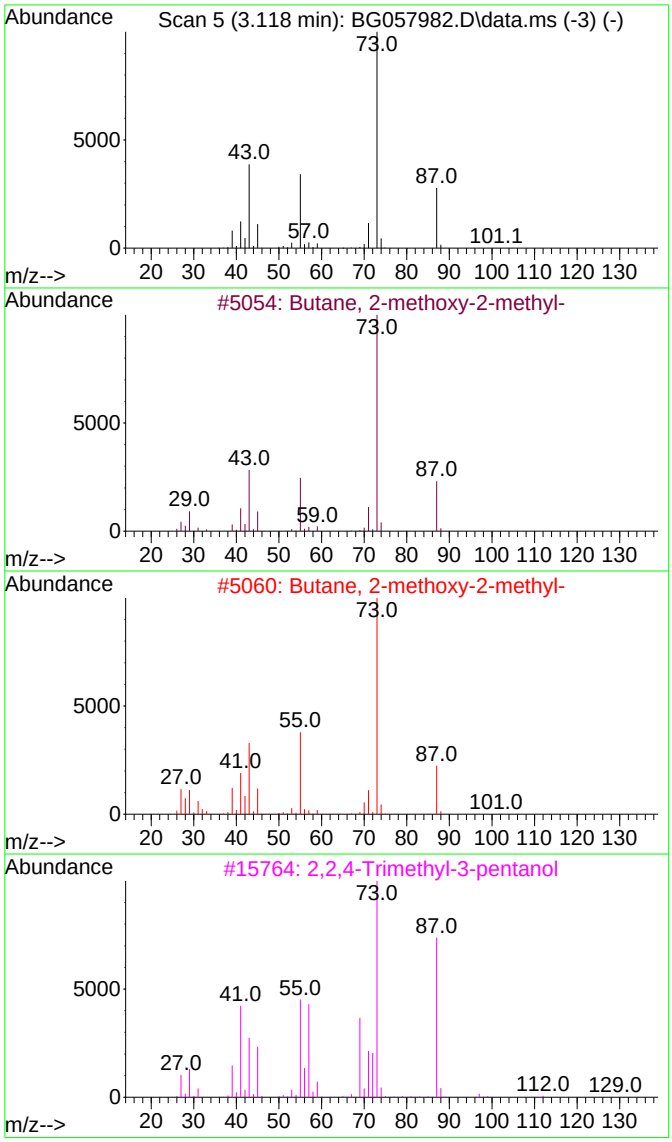
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

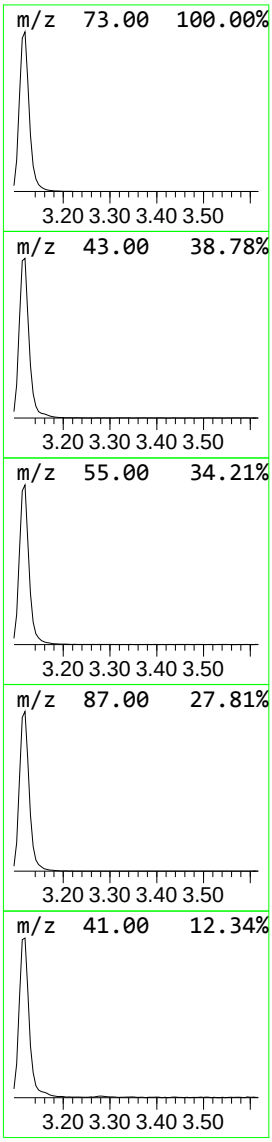
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.118	168.13 ng/ul	2038480	1,4-Dichlorobenzene-d4	7.942

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	28
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

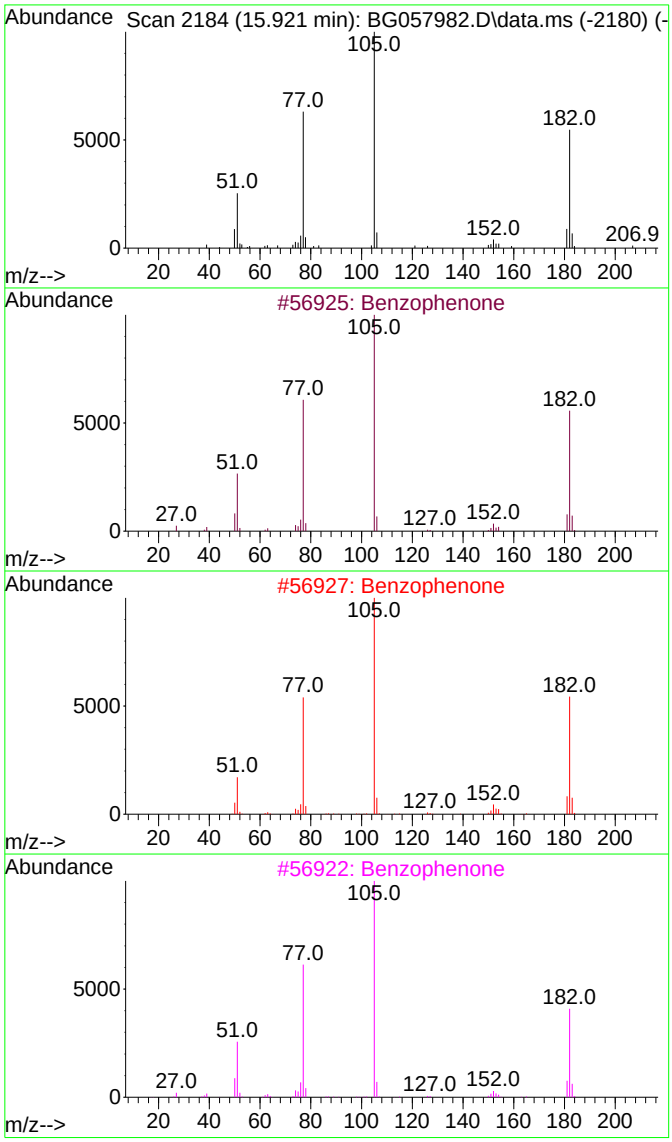
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

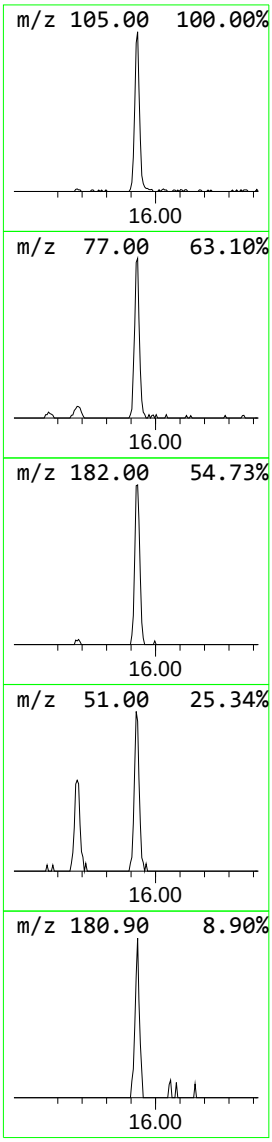
****

Peak Number 2 Benzophenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	2.61 ng/ul	71091	Acenaphthene-d10	14.575

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	Benzophenone	182	C13H10O	000119-61-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

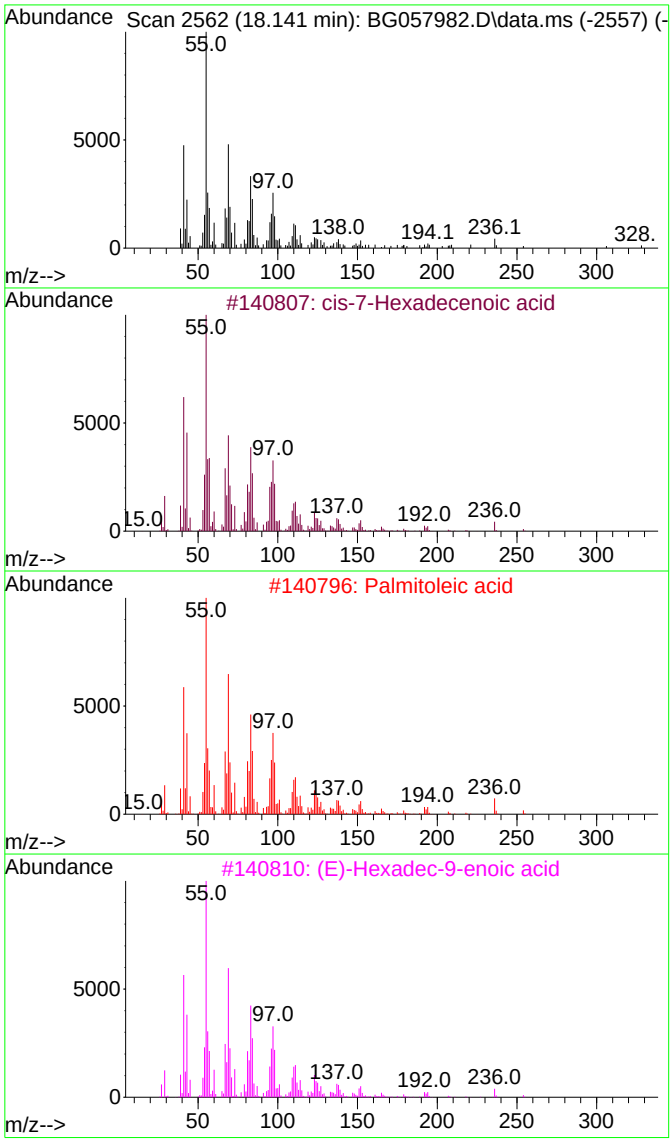
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

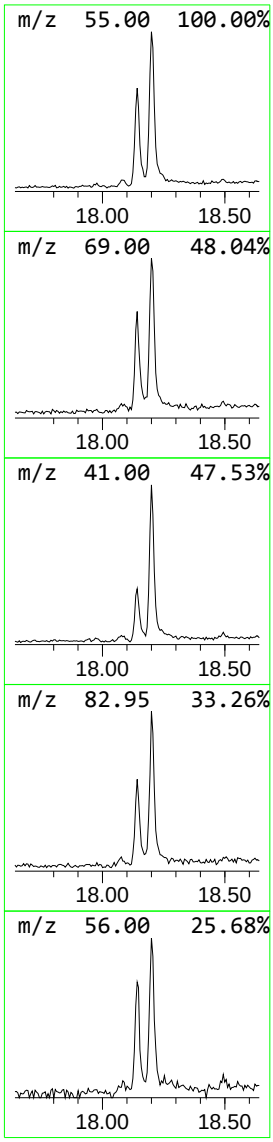
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 cis-7-Hexadecenoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.142	5.21 ng/ul	169237	Phenanthrene-d10	17.319

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	99
2	Palmitoleic acid	254	C16H30O2	000373-49-9	96
3	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	96
4	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	95
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
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Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

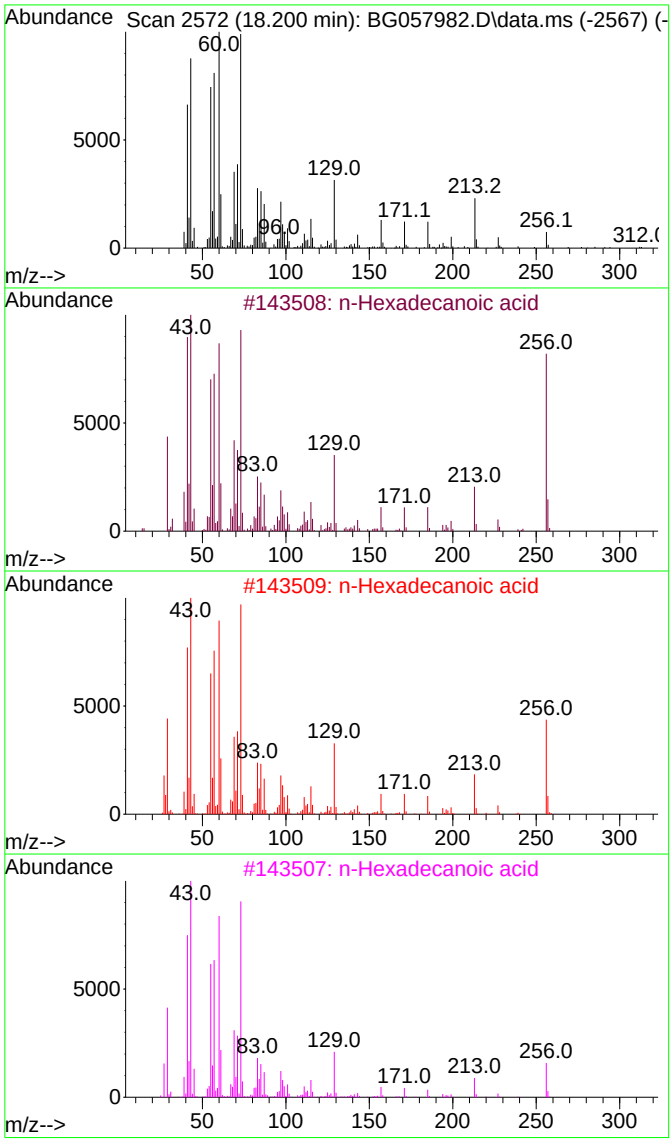
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

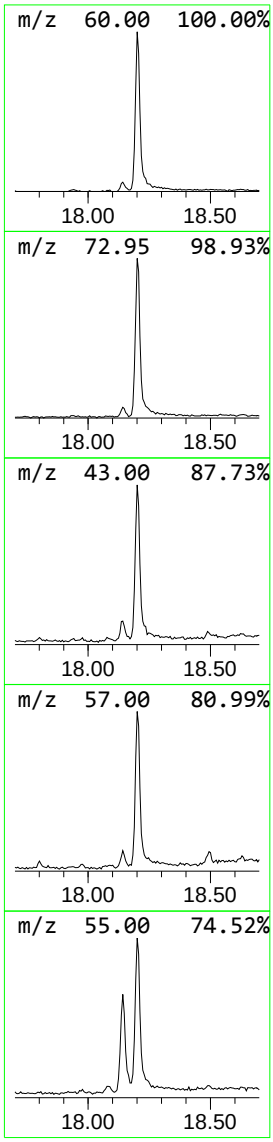
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.200	16.16 ng/ul	524582	Phenanthrene-d10	17.319

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	96
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5	Tridecanoic acid	214	C13H26O2	000638-53-9	90





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Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

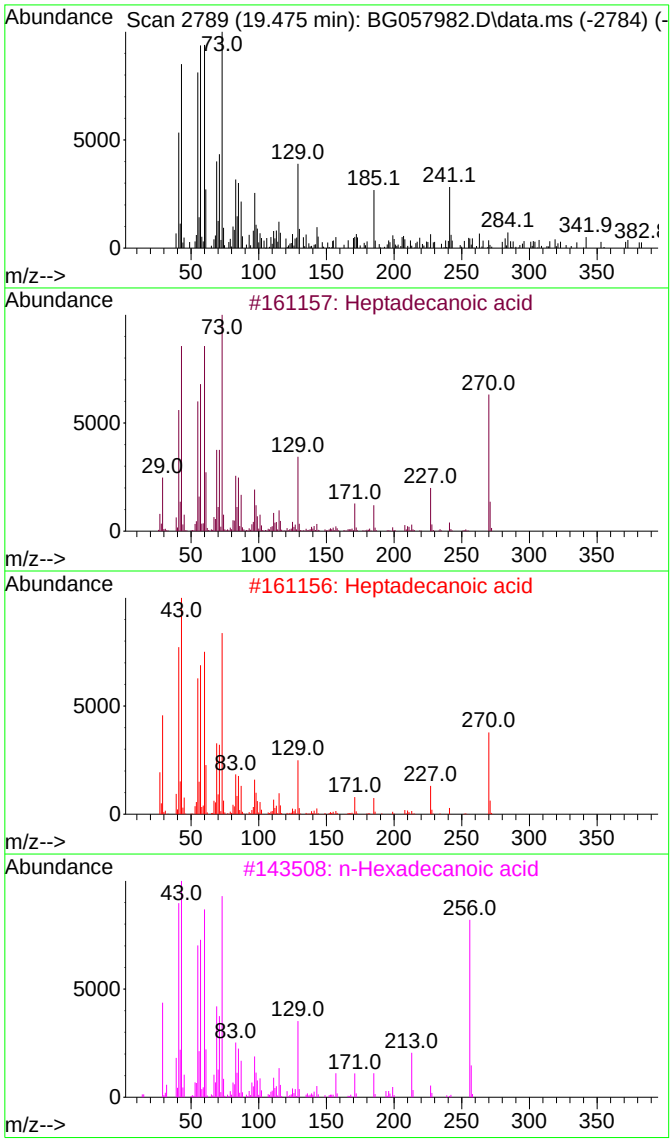
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

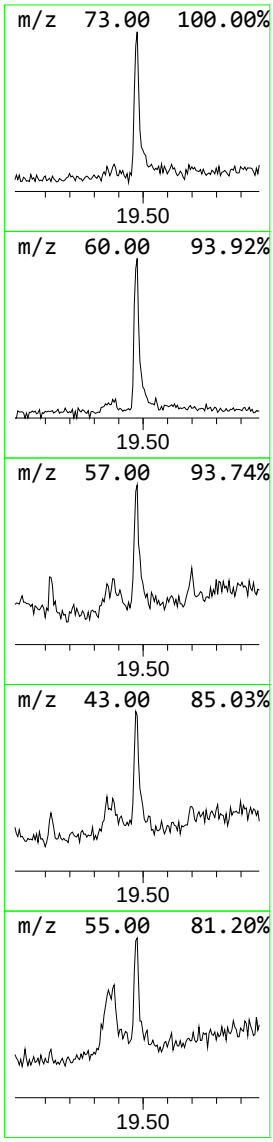
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.475	3.50 ng/ul	108607	Chrysene-d12	21.567

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid	270	C17H34O2	000506-12-7	93
2	Heptadecanoic acid	270	C17H34O2	000506-12-7	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	91





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ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

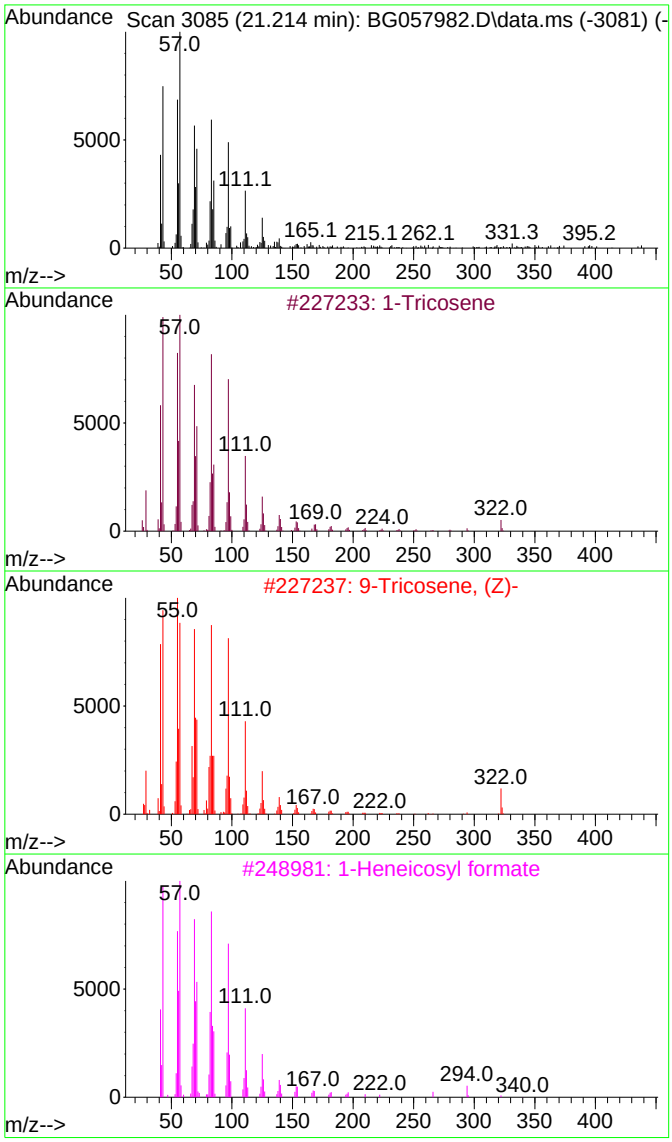
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

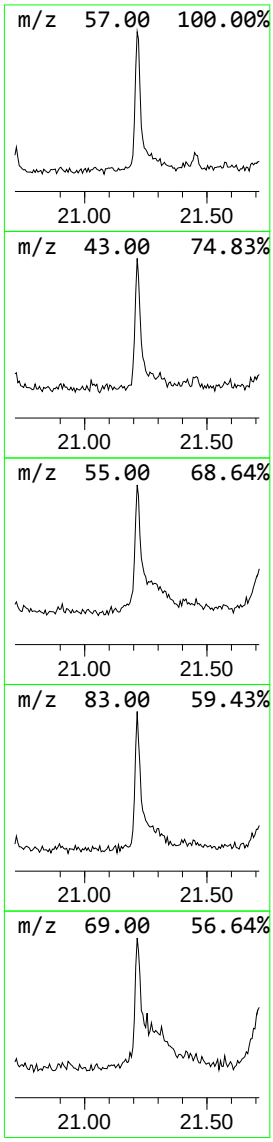
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.214	11.11 ng/ul	344980	Chrysene-d12	21.567

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	94
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91





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Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

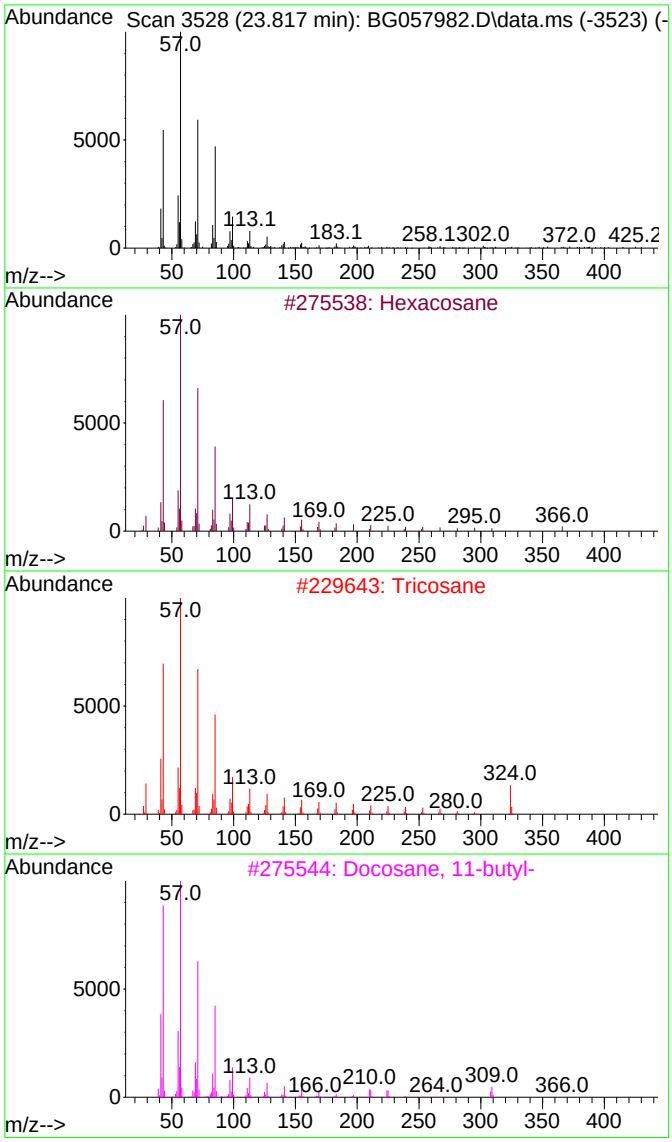
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

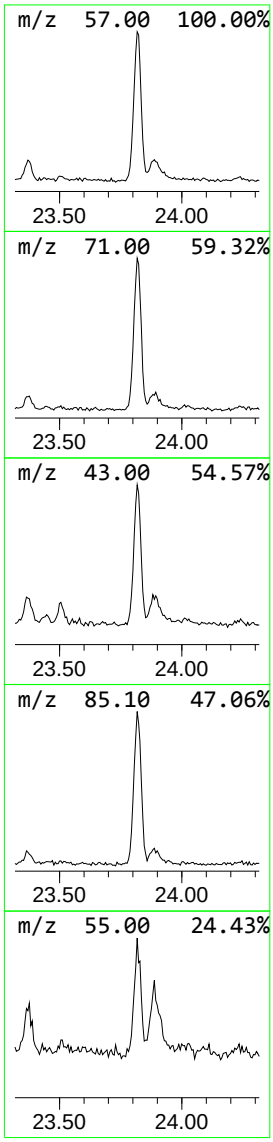
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.817	8.90 ng/ul	341710	Perylene-d12	24.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Tricosane	324	C23H48	000638-67-5	83
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	83
4	Eicosane	282	C20H42	000112-95-8	83
5	Heneicosane	296	C21H44	000629-94-7	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

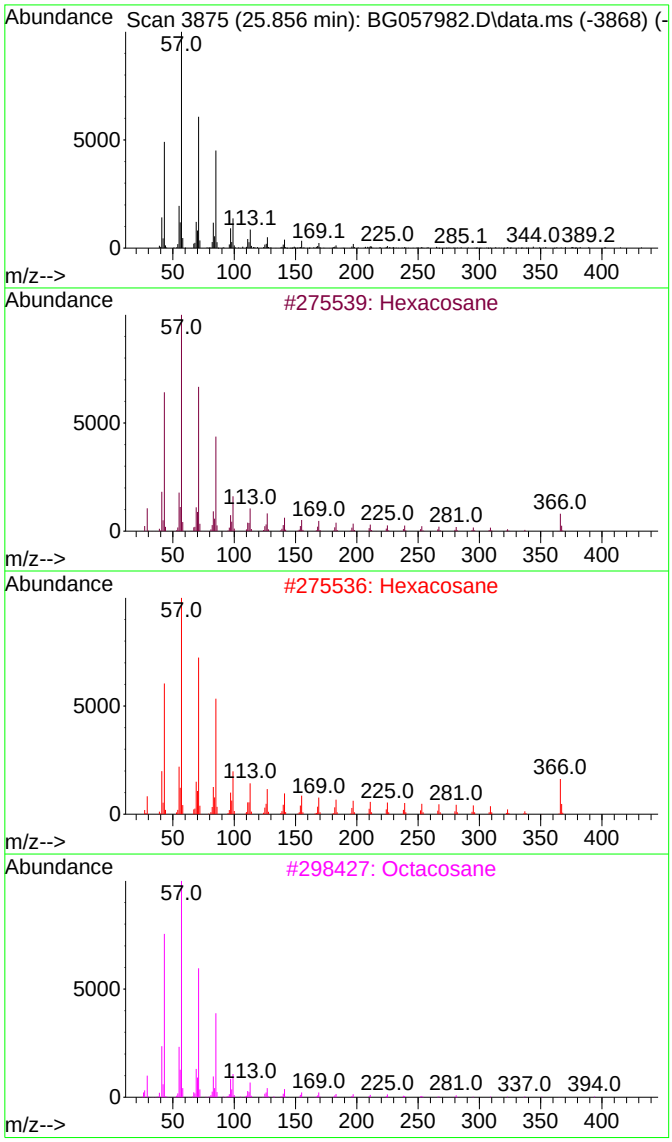
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

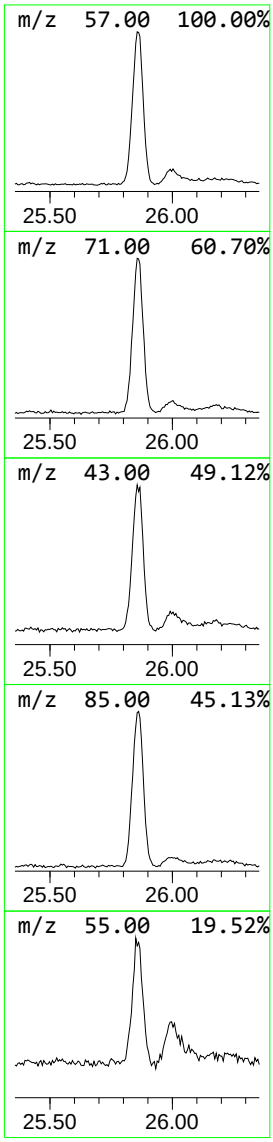
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.856	21.74 ng/ul	834760	Perylene-d12	24.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	92
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90





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Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

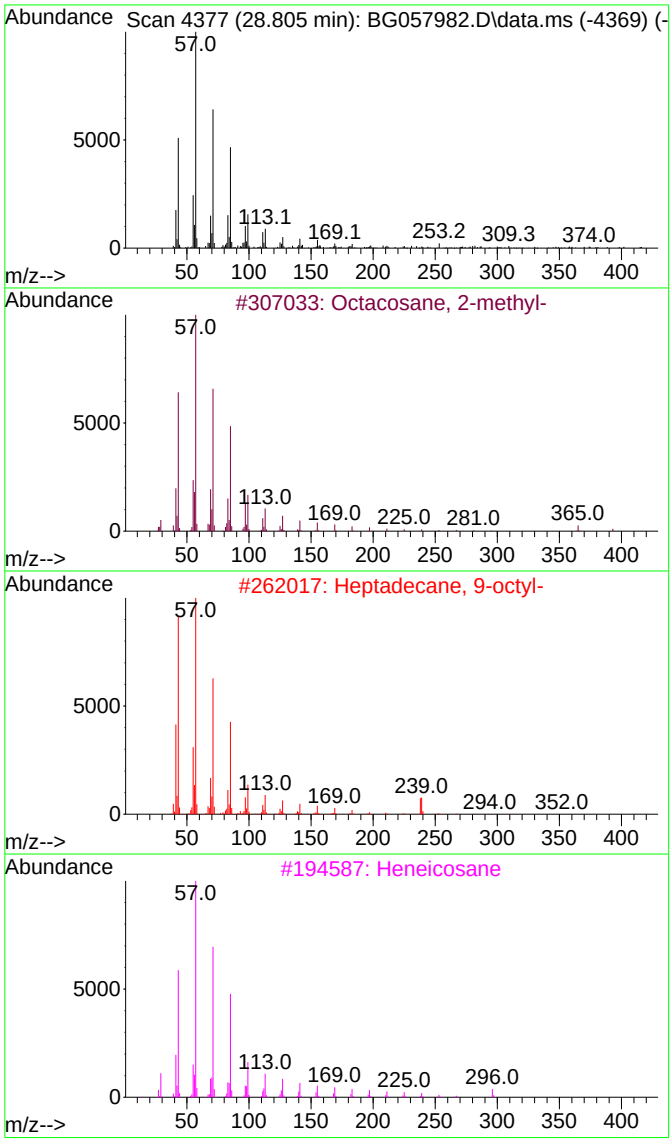
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

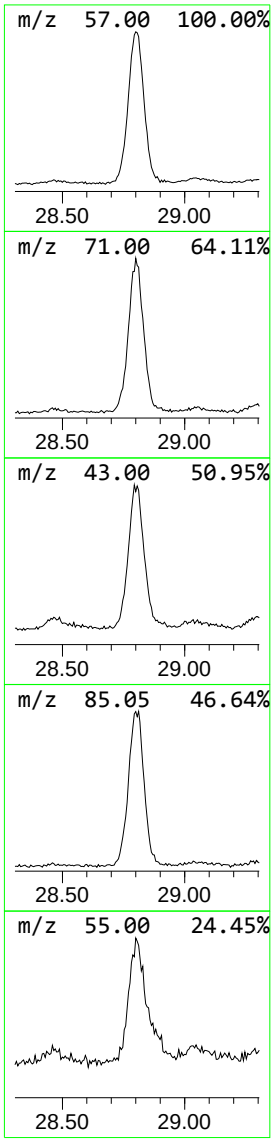
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.805	24.47 ng/ul	939517	Perylene-d12	24.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
5	Heptadecane	240	C17H36	000629-78-7	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

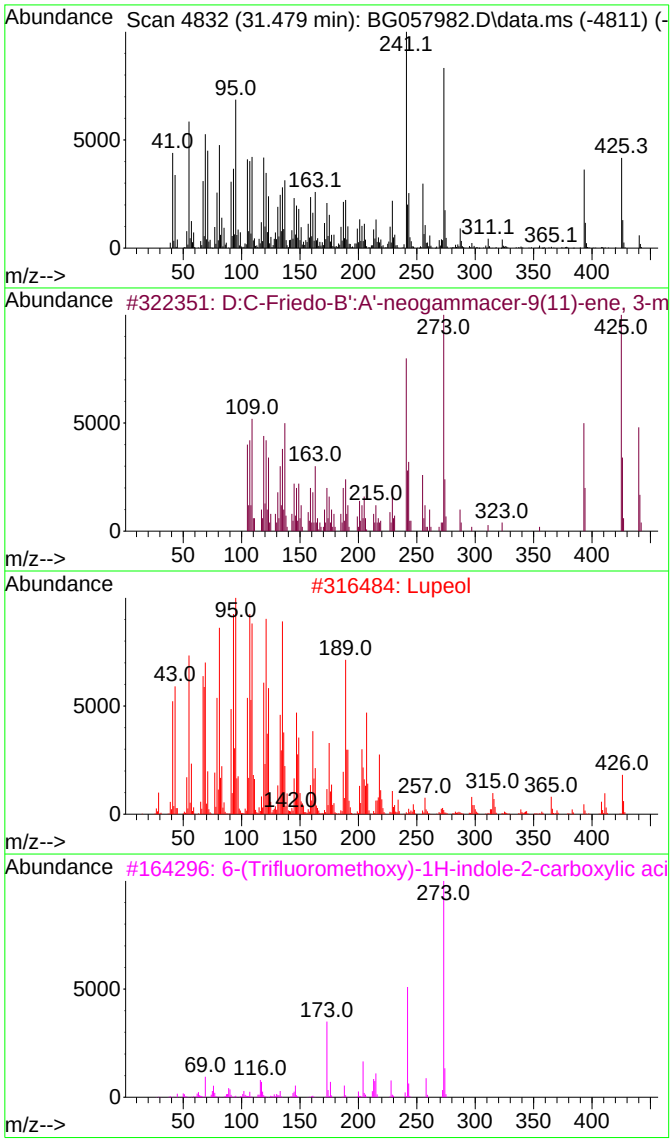
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

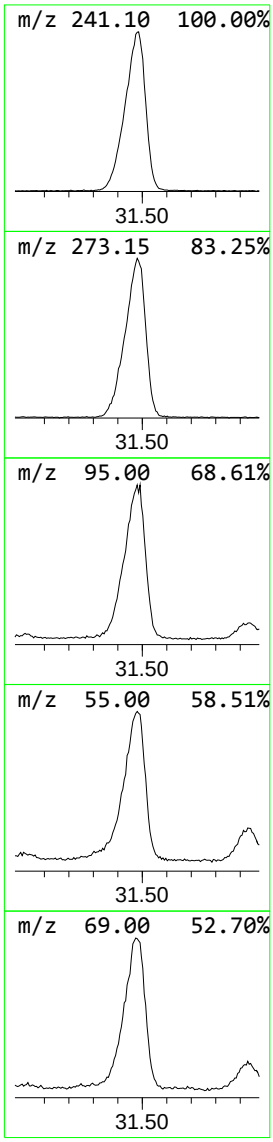
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.479	225.24 ng/ul	8649300	Perylene-d12	24.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	83
2	Lupeol	426	C30H50O	000545-47-1	38
3	6-(Trifluoromethoxy)-1H-indole-2...	273	C12H10F3NO3	1000499-75-7	25
4	Crinan-1-ol, (1.alpha.)-	273	C16H19NO3	041928-89-6	25
5	6-Nitro-2-phenylthieno[2,3-d]pyr...	273	C12H7N3O3S	1000460-07-6	15





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

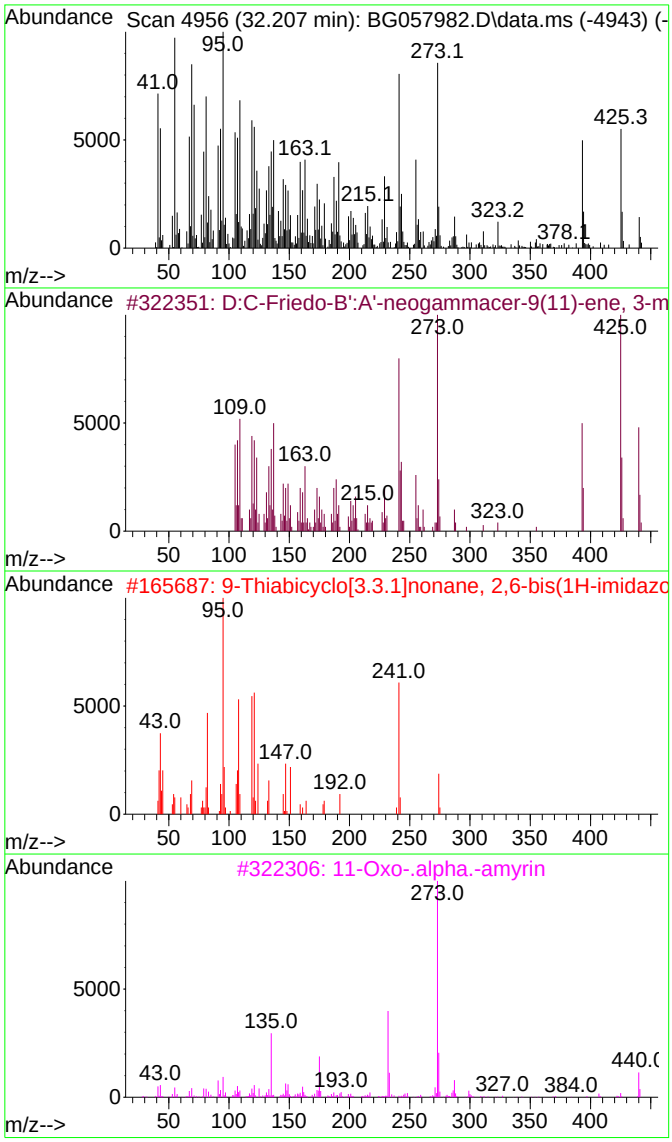
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

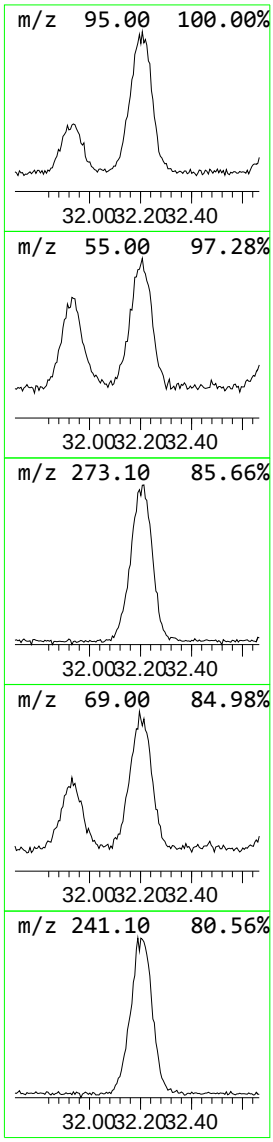
****

Peak Number 11 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
32.207	64.76 ng/ul	2486930	Perylene-d12	24.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	42
2	9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	30
3	11-Oxo-.alpha.-amyrin	440	C30H48O2	002118-90-3	25
4	2-(1H-Indol-3-ylmethylene)-1H-in...	273	C18H11NO2	031060-64-7	25
5	9,19-Cyclolanost-25-en-3-ol, 24-...	440	C31H52O	000511-61-5	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057982.D
Acq On : 4 Jul 2023 10:32
Operator : CG/JU
Sample : 03247-22
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.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
Butane, 2-metho...	3.118	168.1	ng/ul	2038480	1	7.942	242481	20.0
Benzophenone	15.921	2.6	ng/ul	71091	3	14.575	544506	20.0
cis-7-Hexadecen...	18.142	5.2	ng/ul	169237	4	17.319	649123	20.0
n-Hexadecanoic ...	18.200	16.2	ng/ul	524582	4	17.319	649123	20.0
Heptadecanoic acid	19.475	3.5	ng/ul	108607	5	21.567	620894	20.0
(DEL) Alkane: S...	21.214	11.1	ng/ul	344980	5	21.567	620894	20.0
(DEL) Alkane: S...	23.817	8.9	ng/ul	341710	6	24.734	768022	20.0
(DEL) Alkane: S...	25.856	21.7	ng/ul	834760	6	24.734	768022	20.0
(DEL) Alkane: S...	28.805	24.5	ng/ul	939517	6	24.734	768022	20.0
D:C-Friedo-B':A...	31.479	225.2	ng/ul	8649300	6	24.734	768022	20.0
unknown-01	32.207	64.8	ng/ul	2486930	6	24.734	768022	20.0