LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
Acq On : 22 Jun 2023 13:03
Operator : CG/JU
Sample : 03290-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057807.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.625	86	91	101	rBV	73888	108973	4.75%	0.857%
2	4.112	168	174	181	rBV	71016	100254	4.37%	0.789%
3	5.029	323	330	340	rVB	247512	365785	15.94%	2.878%
4	5.428	394	398	403	rBV	19849	29139	1.27%	0.229%
5	5.493	403	409	415	rVV	509142	784500	34.18%	6.172%
6	5.563	415	421	437	rVB2	80579	178689	7.78%	1.406%
7	5.934	478	484	490	rBV2	38599	61404	2.68%	0.483%
8	7.079	671	679	687	rBV	580074	947600	41.28%	7.455%
9	7.919	815	822	828	rBV	103808	172359	7.51%	1.356%
10	9.077	1009	1019	1027	rBV	328506	583587	25.42%	4.591%
11	10.722	1289	1299	1305	rBV	165543	298920	13.02%	2.352%
12	13.178	1709	1717	1727	rVB	967941	1464465	63.80%	11.522%
13	14.553	1941	1951	1957	rBV	306084	477165	20.79%	3.754%
14	15.910	2171	2182	2187	rBV	61482	99650	4.34%	0.784%
15	16.039	2198	2204	2210	rBV	650118	963659	41.98%	7.582%
16	16.263	2238	2242	2251	rBV5	17385	42665	1.86%	0.336%
17	16.621	2291	2303	2306	rBV	35790	68079	2.97%	0.536%
18	16.950	2354	2359	2367	rBV4	19128	33341	1.45%	0.262%
19	17.056	2372	2377	2380	rVV2	20944	30935	1.35%	0.243%
20	17.109	2383	2386	2395	rVB5	16294	29557	1.29%	0.233%
21	17.297	2412	2418	2423	rBV	416255	624321	27.20%	4.912%
22	17.338	2423	2425	2432	rVB	62272	73220	3.19%	0.576%
23	17.491	2444	2451	2455	rBV4	16515	38001	1.66%	0.299%
24	17.579	2462	2466	2468	rBV3	15975	25394	1.11%	0.200%
25	17.602	2468	2470	2475	rVB3	26304	39627	1.73%	0.312%
26	17.790	2499	2502	2505	rBV3	23188	24735	1.08%	0.195%
27	17.878	2513	2517	2525	rVB2	29739	49049	2.14%	0.386%
28	18.184	2563	2569	2572	rBV2	89496	173755	7.57%	1.367%
29	18.219	2572	2575	2581	rVB	95696	141009	6.14%	1.109%
30	18.354	2594	2598	2603	rVV3	32701	49755	2.17%	0.391%
31	18.401	2603	2606	2610	rVB3	21056	29145	1.27%	0.229%
32	18.484	2616	2620	2624	rBV2	42162	60503	2.64%	0.476%
33	18.566	2630	2634	2639	rVB3	18363	27940	1.22%	0.220%
34	18.672	2648	2652	2656	rBV2	38177	53416	2.33%	0.420%
35	19.006	2706	2709	2713	rVB	22702	25970	1.13%	0.204%
36	19.089	2719	2723	2725	rBV	36702	45372	1.98%	0.357%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
Acq On : 22 Jun 2023 13:03
Operator : CG/JU
Sample : 03290-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.118	2725	2728	2730	rVV	22053	23064	1.00%	0.181%
38	19.224	2743	2746	2752	rBV5	20299	30014	1.31%	0.236%
39	19.347	2763	2767	2774	rVB2	74662	109180	4.76%	0.859%
40	19.412	2775	2778	2781	rBV2	37739	45151	1.97%	0.355%
41	19.459	2782	2786	2789	rBV6	31233	40684	1.77%	0.320%
42	19.694	2823	2826	2827	rBV	38702	44659	1.95%	0.351%
43	19.864	2851	2855	2857	rBV3	42004	59283	2.58%	0.466%
44	19.917	2858	2864	2869	rVB	1714264	2295465	100.00%	18.059%
45	20.223	2914	2916	2921	rVB2	51614	53335	2.32%	0.420%
46	20.716	2997	3000	3003	rBV	46564	51765	2.26%	0.407%
47	21.204	3080	3083	3092	rVB3	165394	250287	10.90%	1.969%
48	21.551	3136	3142	3147	rBV2	383911	660108	28.76%	5.193%
49	24.700	3670	3678	3694	rVB	241427	725678	31.61%	5.709%

Sum of corrected areas: 12710611

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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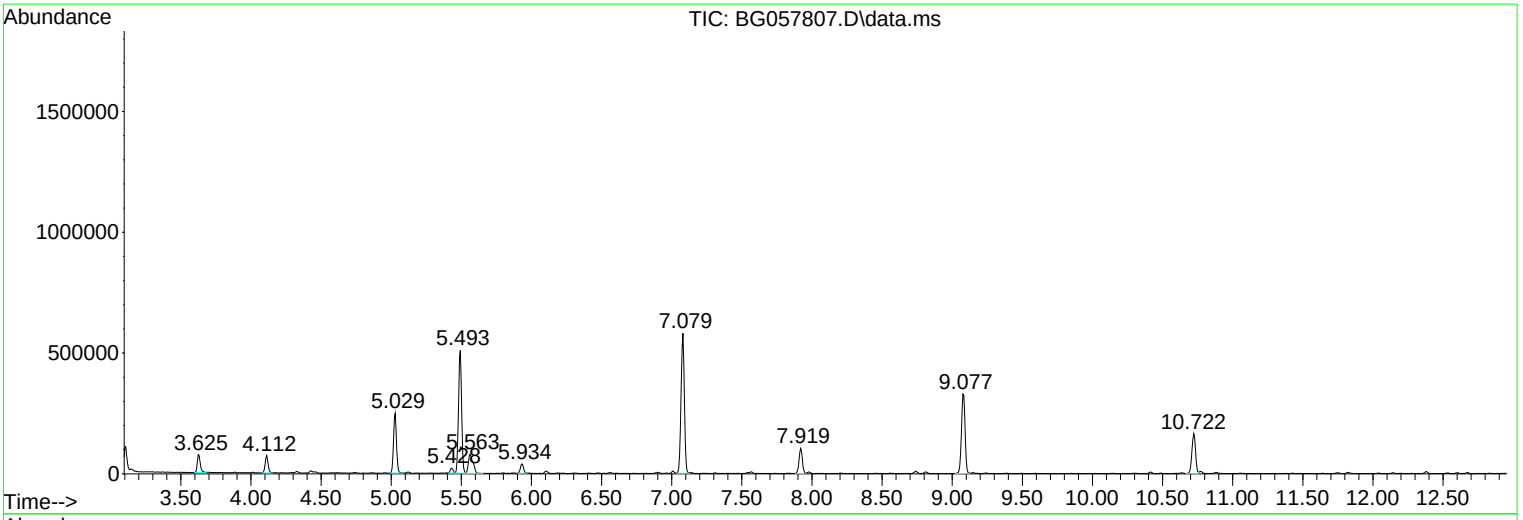
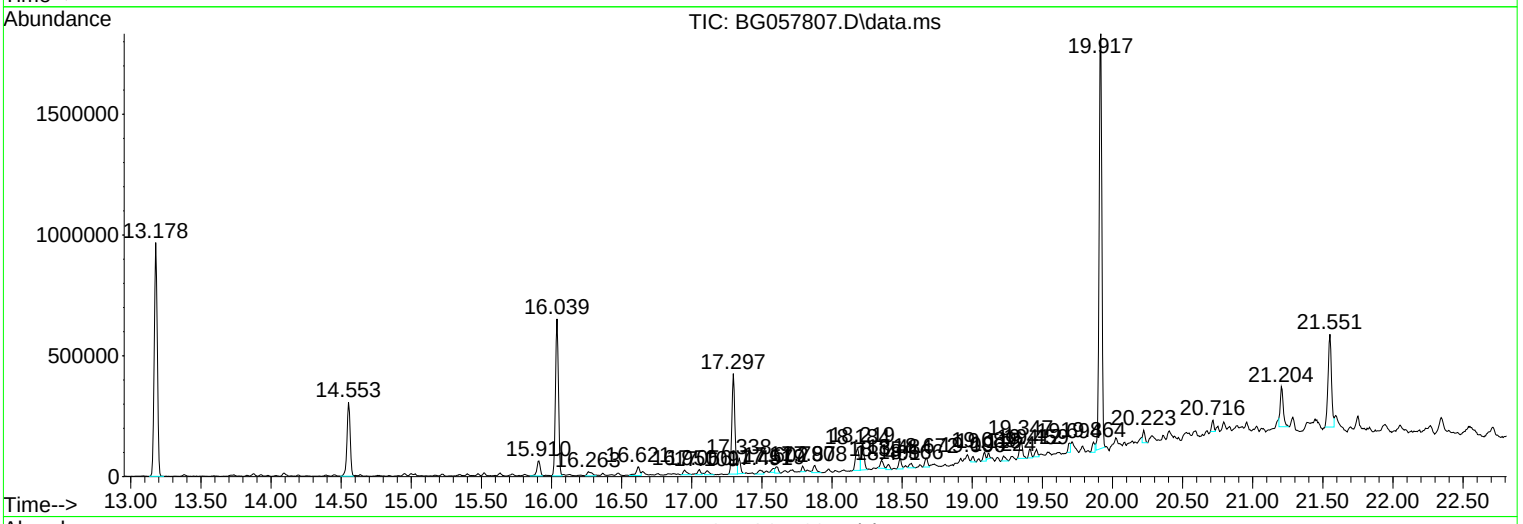
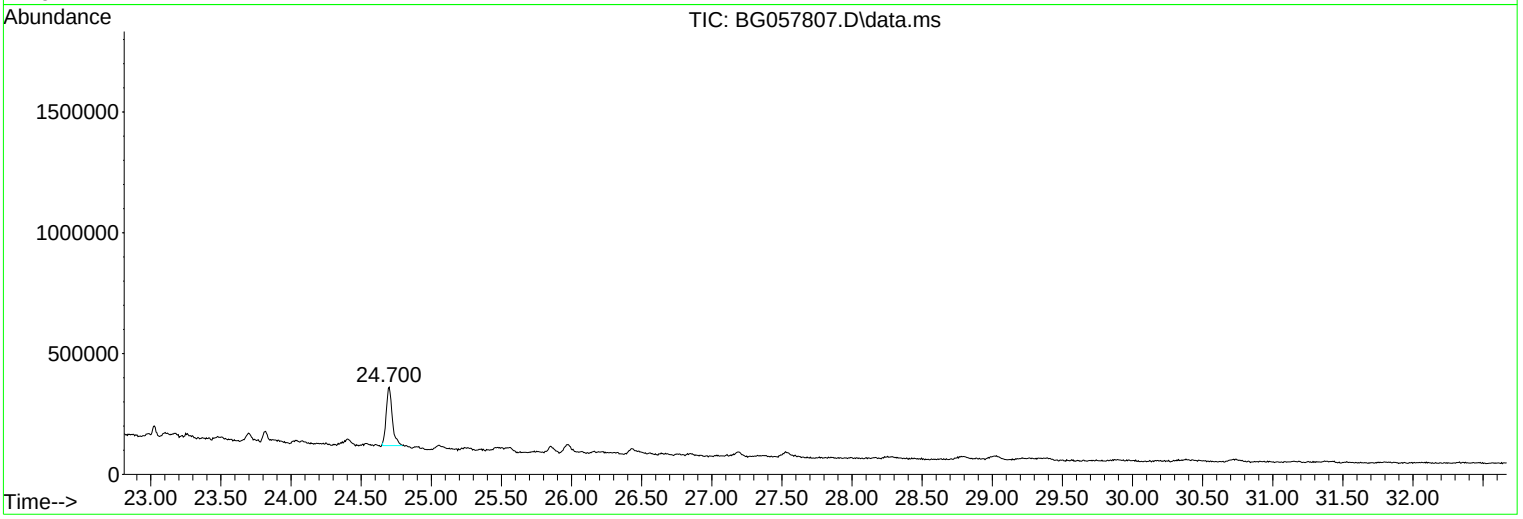
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
Acq On : 22 Jun 2023 13:03
Operator : CG/JU
Sample : 03290-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

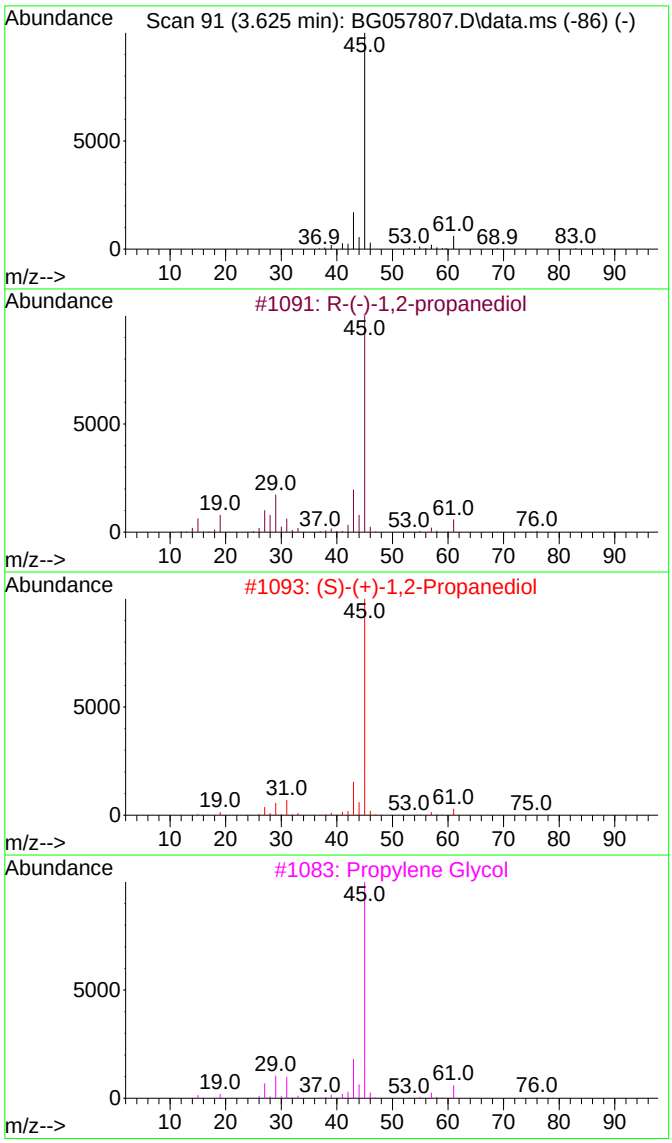
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

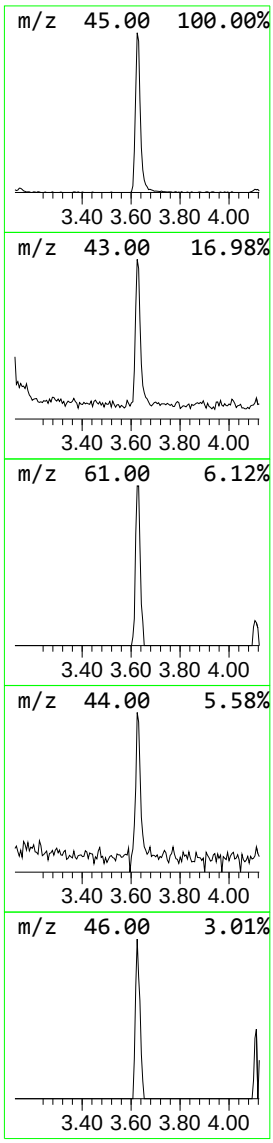
****

Peak Number 1 unknown3.625 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.625	12.64 ng	108973	1,4-Dichlorobenzene-d4	7.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	43
4	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
Acq On : 22 Jun 2023 13:03
Operator : CG/JU
Sample : 03290-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

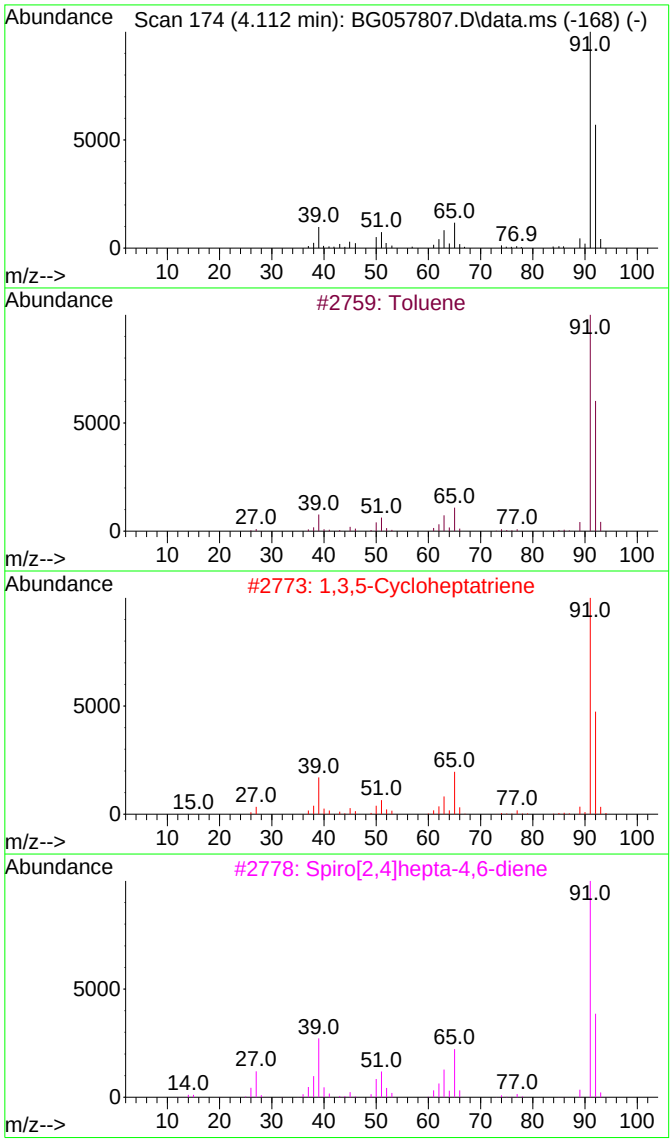
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

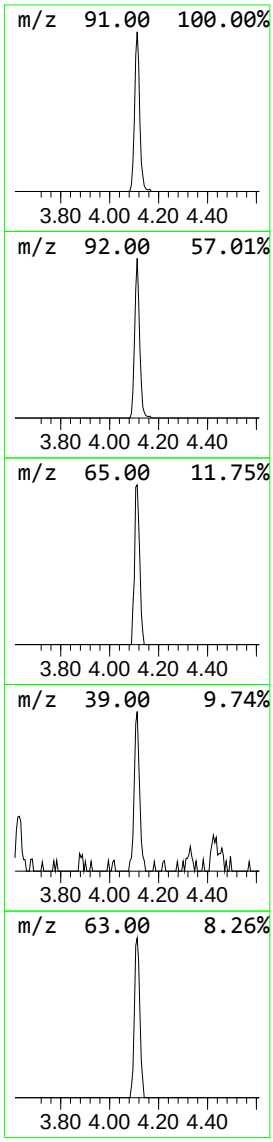
****

Peak Number 2 1,3,5-Cycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.112	11.63 ng	100254	1,4-Dichlorobenzene-d4	7.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	94
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
3	Spiro[2,4]hepta-4,6-diene	92	C7H8	000765-46-8	87
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	64
5	2,5-Norbornadiene	92	C7H8	000121-46-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
Acq On : 22 Jun 2023 13:03
Operator : CG/JU
Sample : 03290-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

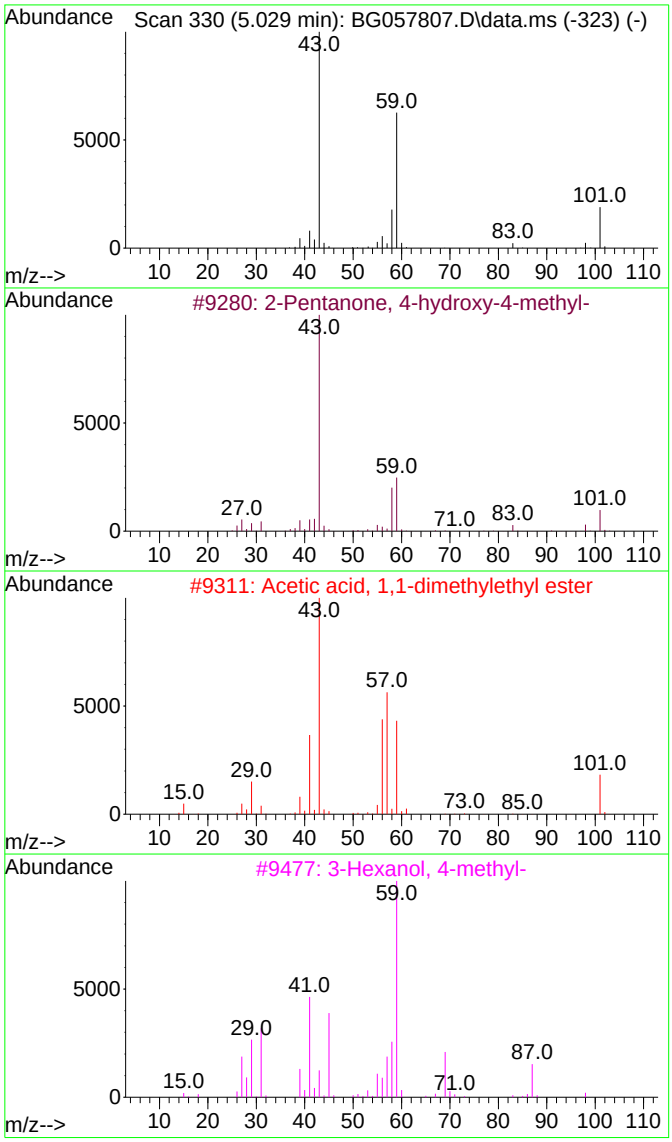
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

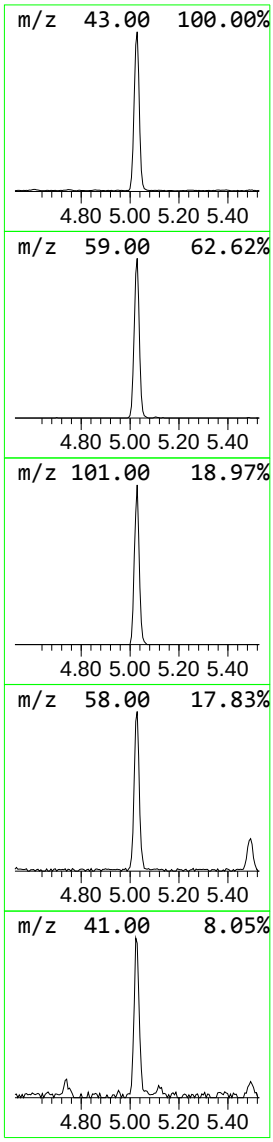
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.029	42.44 ng	365785	1,4-Dichlorobenzene-d4	7.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
Acq On : 22 Jun 2023 13:03
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Sample : 03290-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

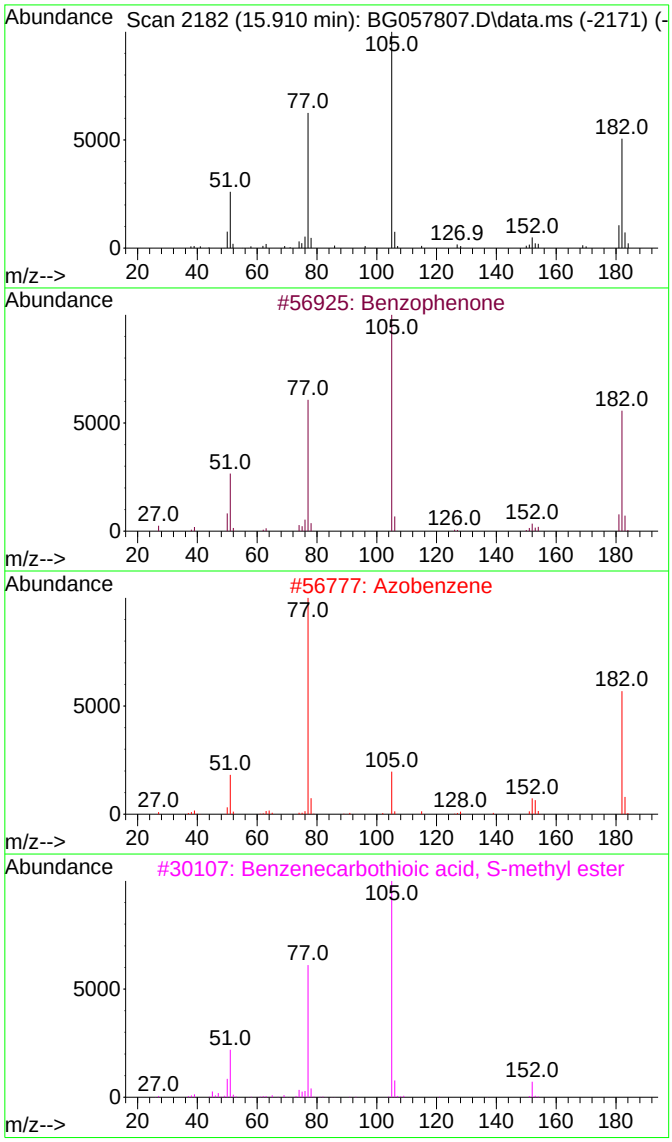
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

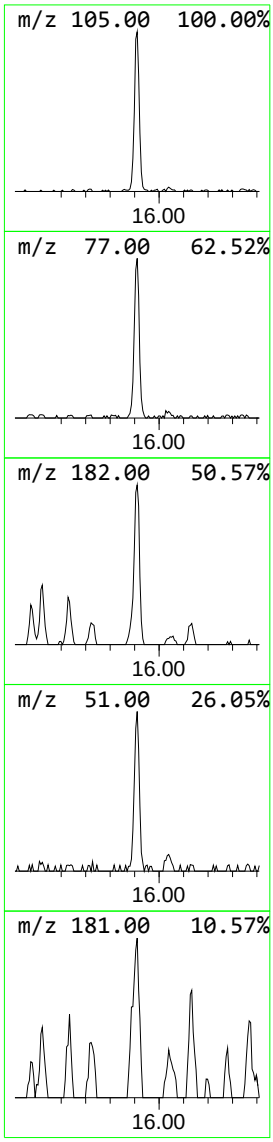
****

Peak Number 7 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.910	4.18 ng	99650	Acenaphthene-d10	14.553

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	58
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
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Operator : CG/JU
Sample : 03290-01
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

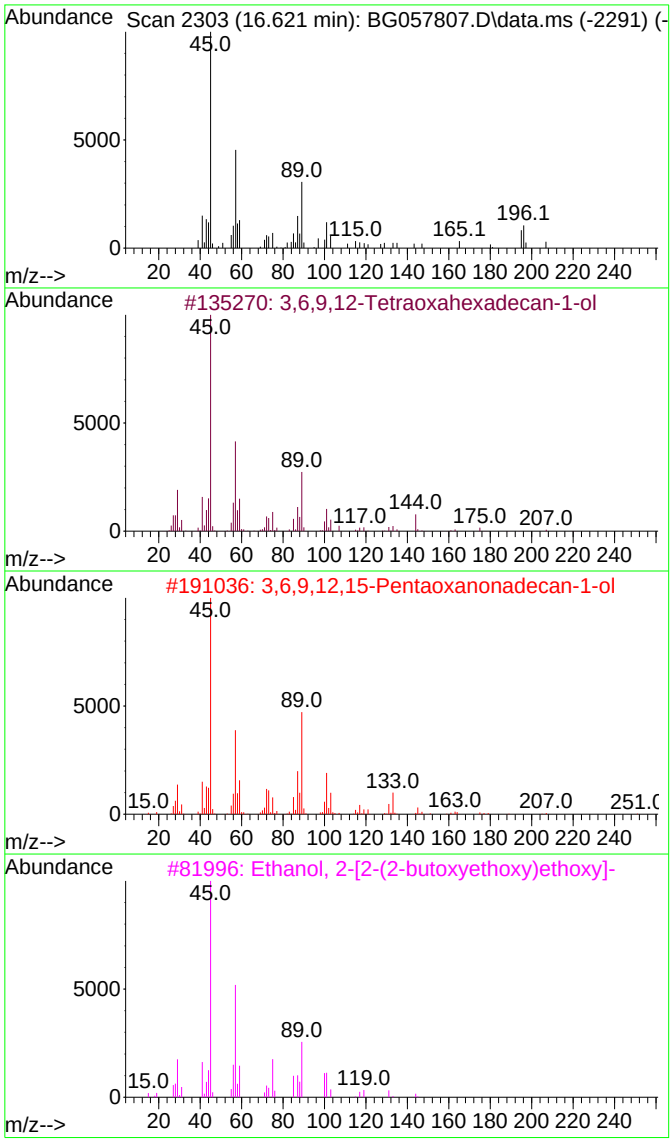
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

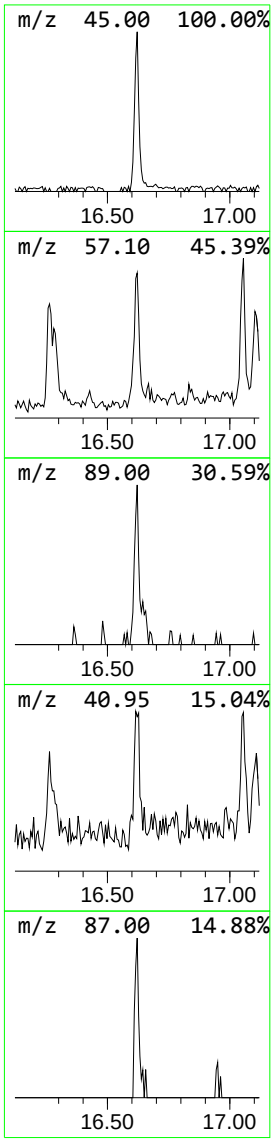
****

Peak Number 8 3,6,9,12-Tetraoxahexadecan-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.621	2.18 ng	68079	Phenanthrene-d10	17.297

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	87
2	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	80
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	80
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	72
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	72





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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

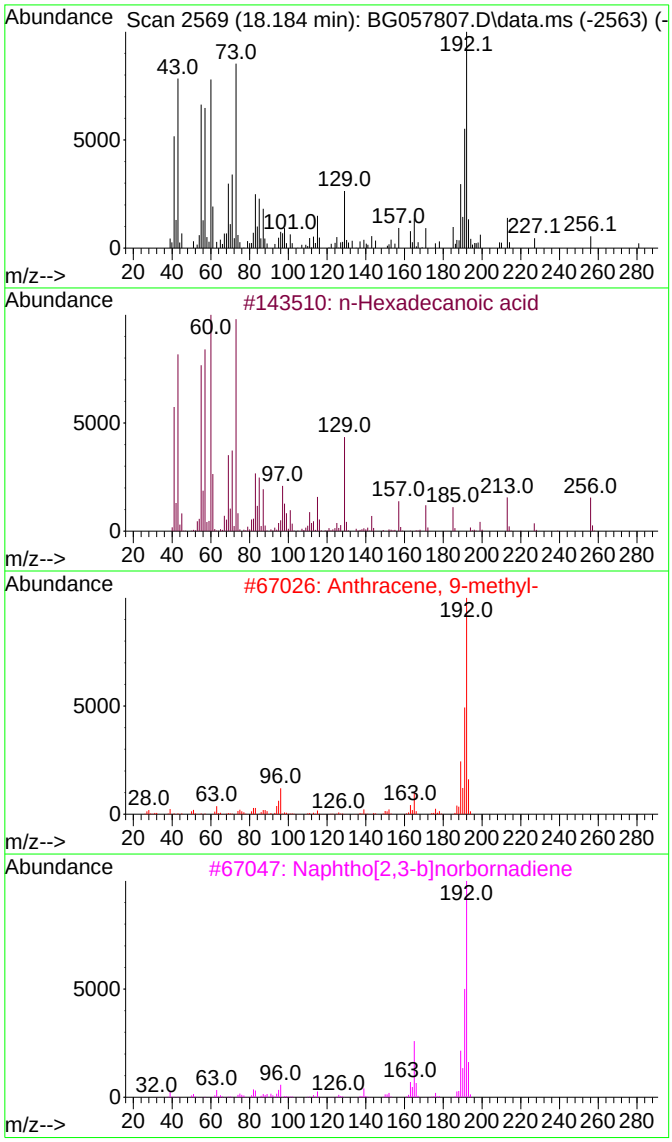
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

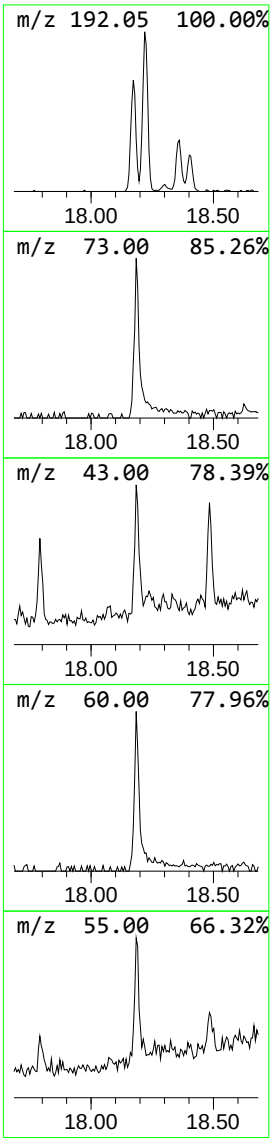
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.184	5.57 ng	173755	Phenanthrene-d10	17.297

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	70
3	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	51
4	Tridecanoic acid	214	C13H26O2	000638-53-9	46
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
Acq On : 22 Jun 2023 13:03
Operator : CG/JU
Sample : 03290-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

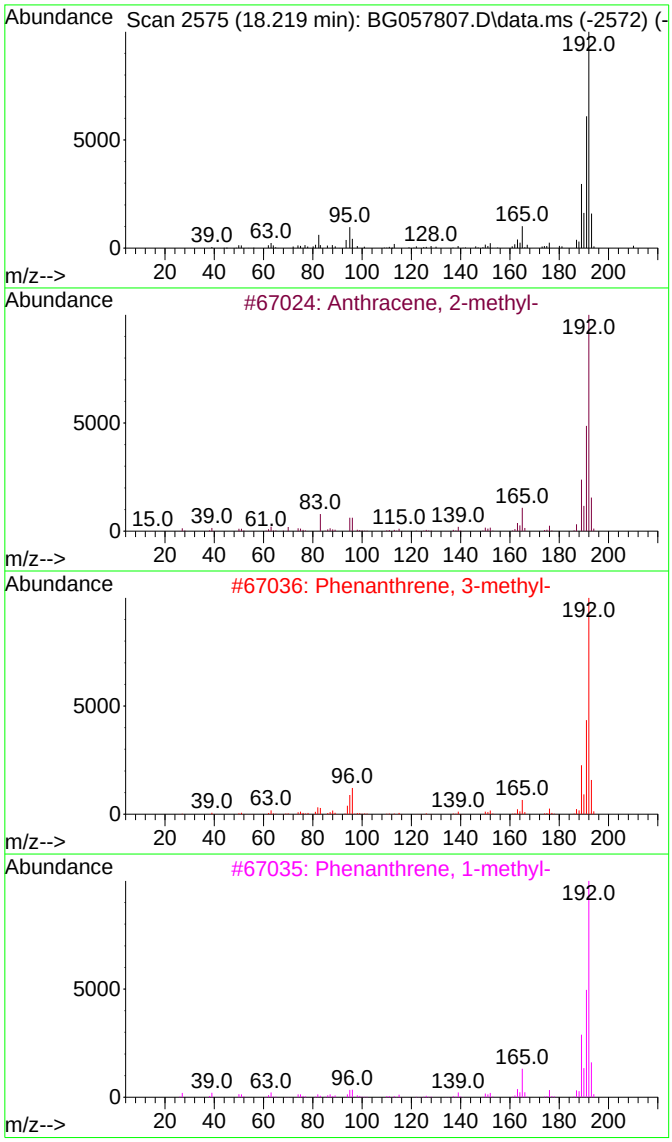
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

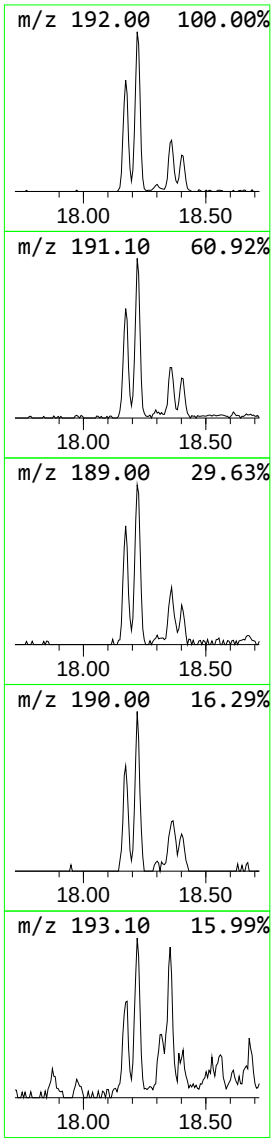
****

Peak Number 10 Anthracene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.219	4.52 ng	141009	Phenanthrene-d10	17.297

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
2	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	91
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
Acq On : 22 Jun 2023 13:03
Operator : CG/JU
Sample : 03290-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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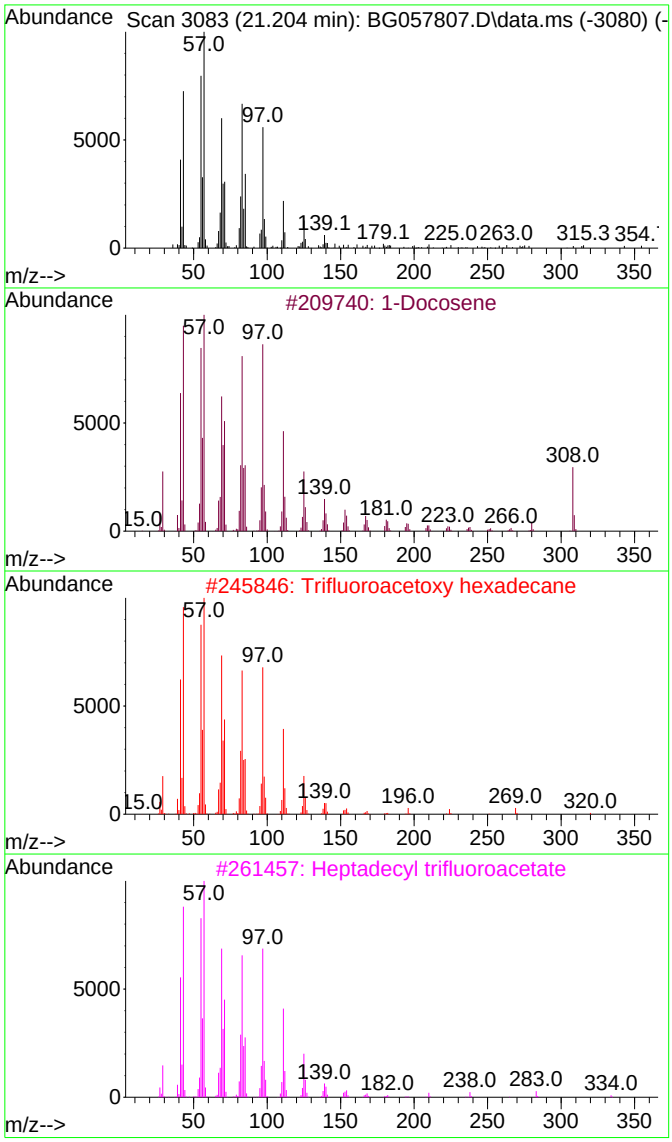
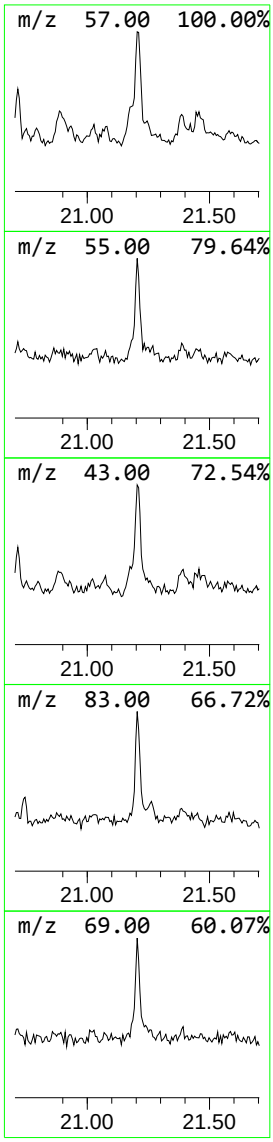
Peak Number 12 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.204	7.58 ng	250287	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057807.D
Acq On : 22 Jun 2023 13:03
Operator : CG/JU
Sample : 03290-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
unknown3.625	3.625	12.6	ng	108973	1	7.919	172359	20.0
1,3,5-Cycloheptatrie...	4.112	11.6	ng	100254	1	7.919	172359	20.0
2-Pentanone, 4-...	5.029	42.4	ng	365785	1	7.919	172359	20.0
Benzophenone	15.910	4.2	ng	99650	3	14.553	477165	20.0
3,6,9,12-Tetraoxatetr...	16.621	2.2	ng	68079	4	17.297	624321	20.0
n-Hexadecanoic ...	18.184	5.6	ng	173755	4	17.297	624321	20.0
Anthracene, 2-m...	18.219	4.5	ng	141009	4	17.297	624321	20.0
1-Docosene	21.204	7.6	ng	250287	5	21.551	660108	20.0