LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056306.D
Acq On : 16 Jan 2023 21:35
Operator : CG/JU
Sample : 01132-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-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-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056306.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.329	3	7	20	rVB	145771	226428	7.99%	1.683%
2	5.356	344	352	360	rBV	127433	200616	7.08%	1.492%
3	5.832	426	433	444	rBV	562782	919627	32.45%	6.837%
4	7.448	697	708	717	rBV	563846	996232	35.15%	7.407%
5	8.318	847	856	864	rBV	142435	248591	8.77%	1.848%
6	9.487	1047	1055	1063	rBV	325748	580806	20.49%	4.318%
7	11.144	1330	1337	1345	rBV	197917	349329	12.33%	2.597%
8	13.553	1740	1747	1757	rVB	1203143	1849184	65.24%	13.748%
9	14.927	1973	1981	1988	rBV	360499	567109	20.01%	4.216%
10	16.261	2202	2208	2217	rBV	304231	439685	15.51%	3.269%
11	16.408	2226	2233	2245	rBV	795526	1291234	45.56%	9.600%
12	16.590	2258	2264	2271	rBV	43772	68646	2.42%	0.510%
13	17.665	2439	2447	2452	rBV	485203	756976	26.71%	5.628%
14	18.506	2584	2590	2596	rBV4	55585	97269	3.43%	0.723%
15	19.692	2787	2792	2798	rVB	43393	66898	2.36%	0.497%
16	20.051	2850	2853	2858	rVB2	50221	70030	2.47%	0.521%
17	20.239	2879	2885	2891	rBV	2244323	2834257	100.00%	21.072%
18	21.537	3102	3106	3116	rBV2	85867	150802	5.32%	1.121%
19	21.954	3170	3177	3184	rBV2	466963	798356	28.17%	5.936%
20	23.711	3472	3476	3482	rVB2	44544	90191	3.18%	0.671%
21	25.403	3753	3764	3775	rBV3	274033	847846	29.91%	6.304%

Sum of corrected areas: 13450112

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Misc :
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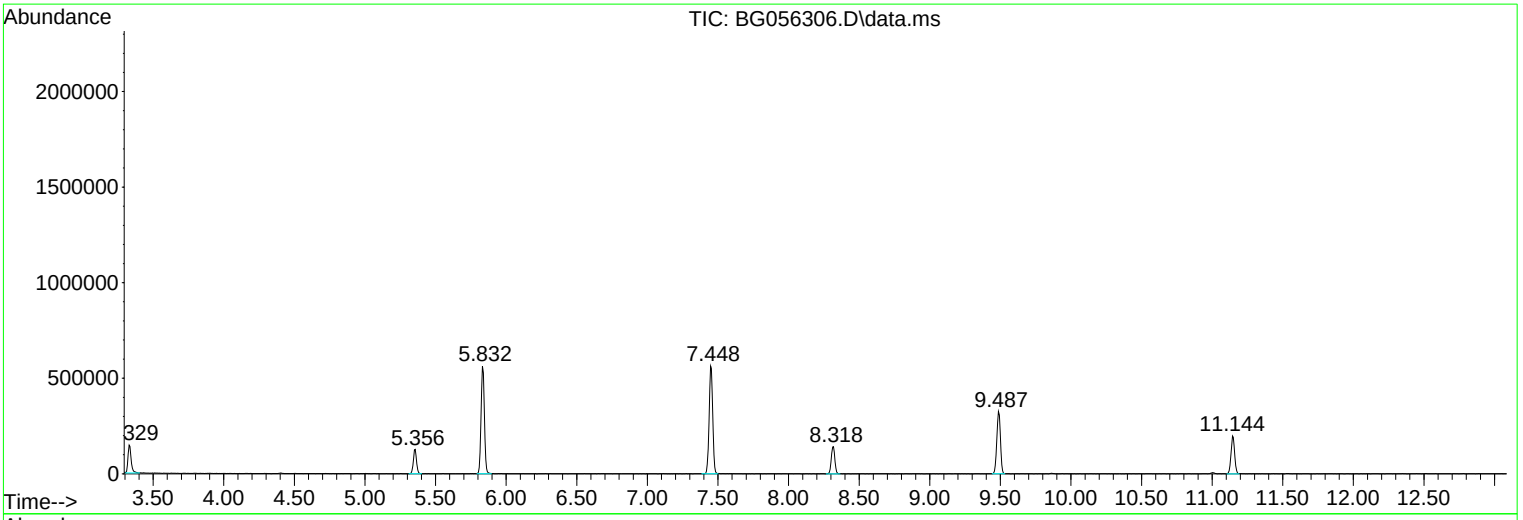
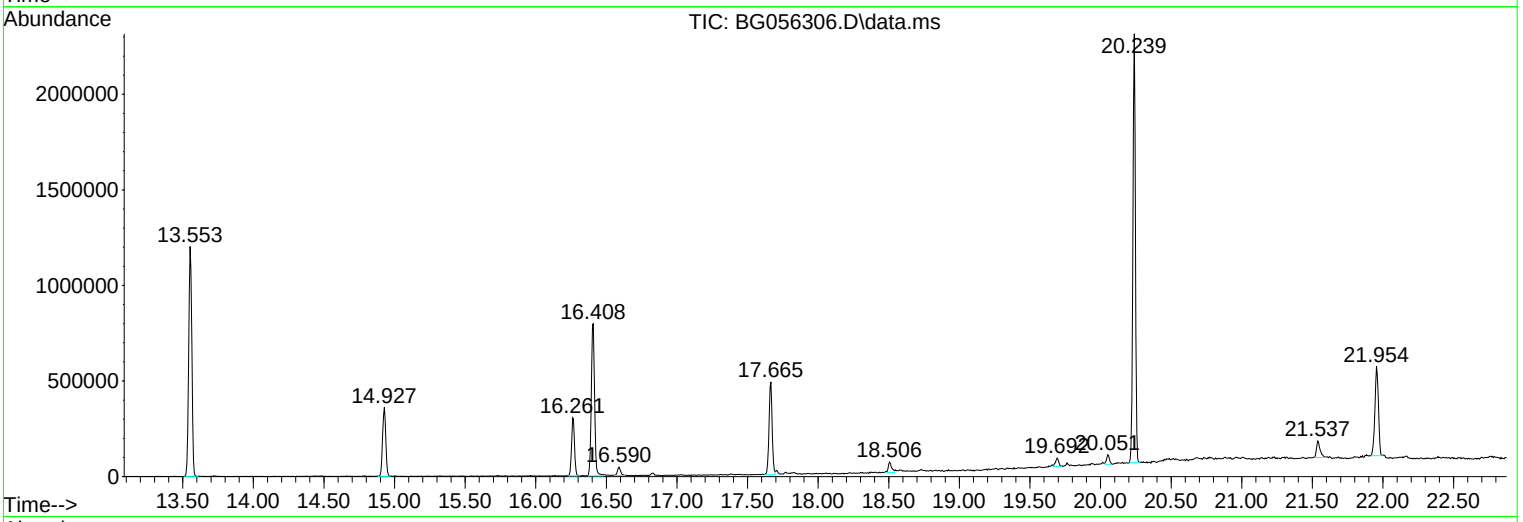
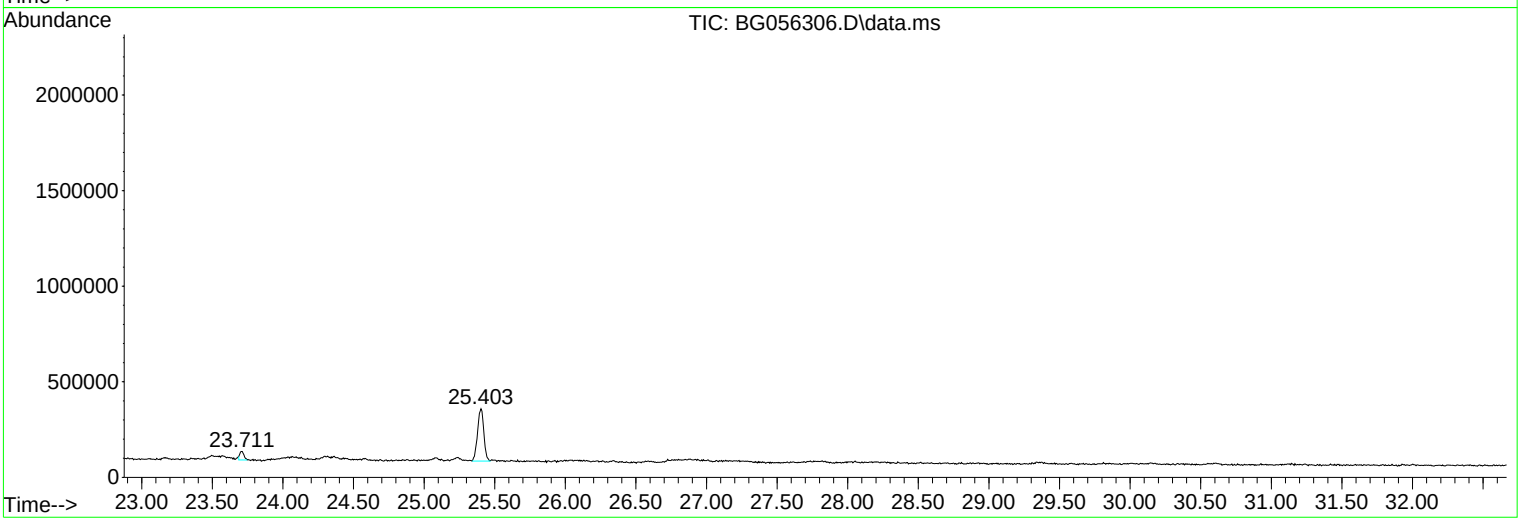
Instrument :
BNA_G
ClientSampleId :
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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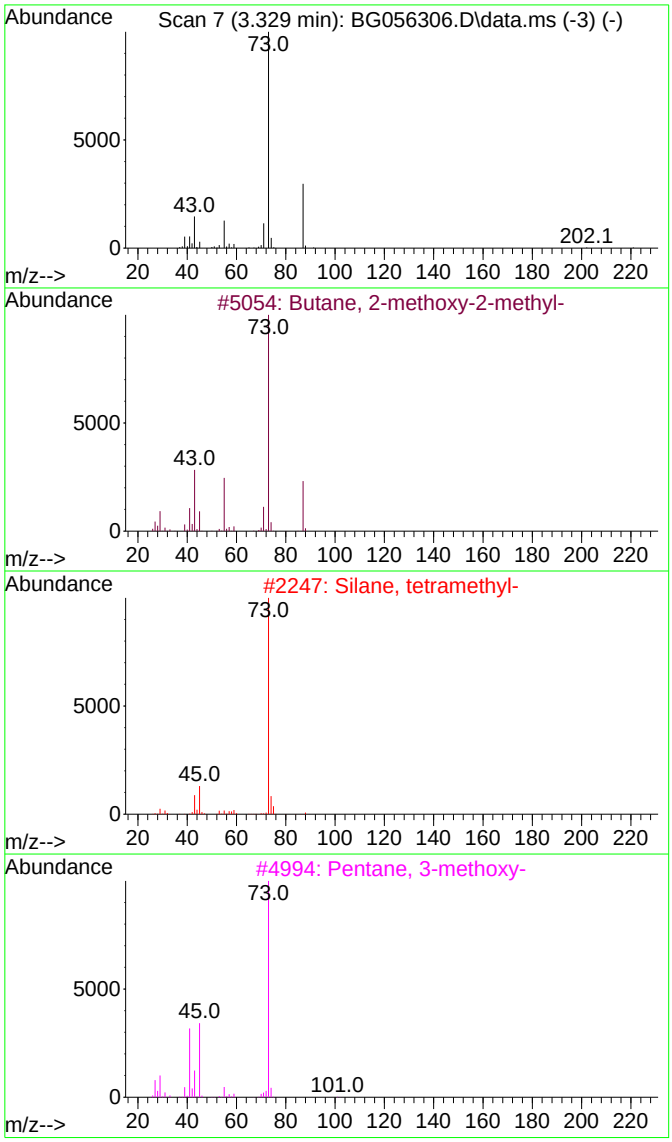
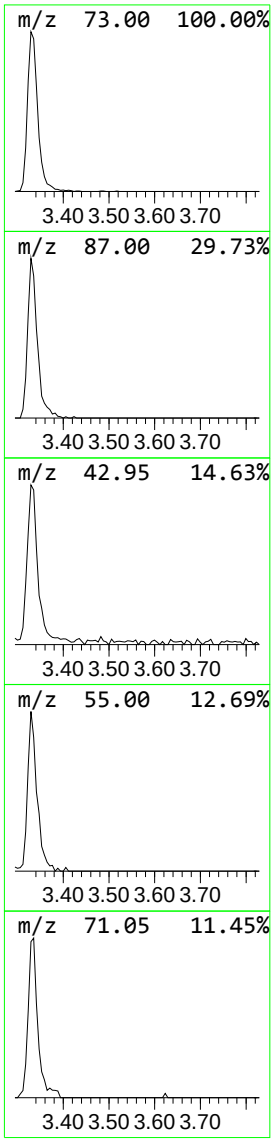
Peak Number 1 unknown3.329 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.329	18.22 ng	226428	1,4-Dichlorobenzene-d4	8.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	38
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	9
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9





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Operator : CG/JU
Sample : 01132-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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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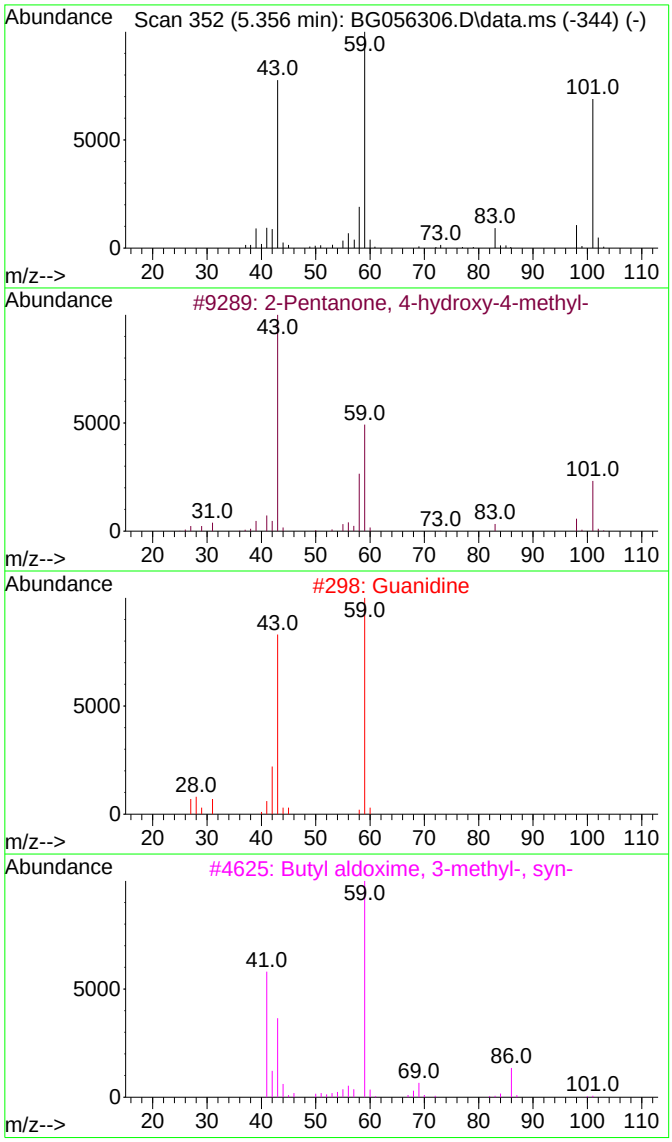
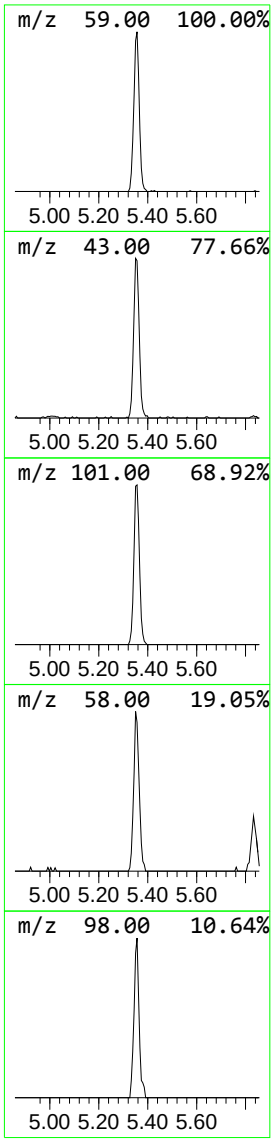
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.356	16.14 ng	200616	1,4-Dichlorobenzene-d4	8.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Guanidine	59	CH5N3	000113-00-8	37
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	35
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
5	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	25





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Operator : CG/JU
Sample : 01132-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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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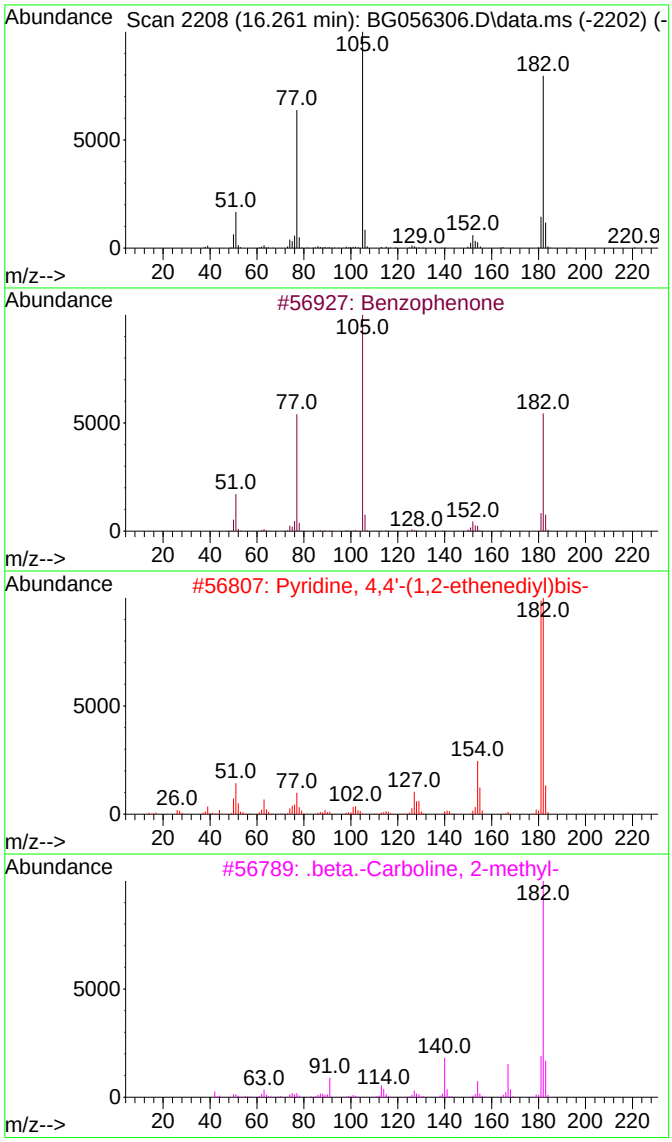
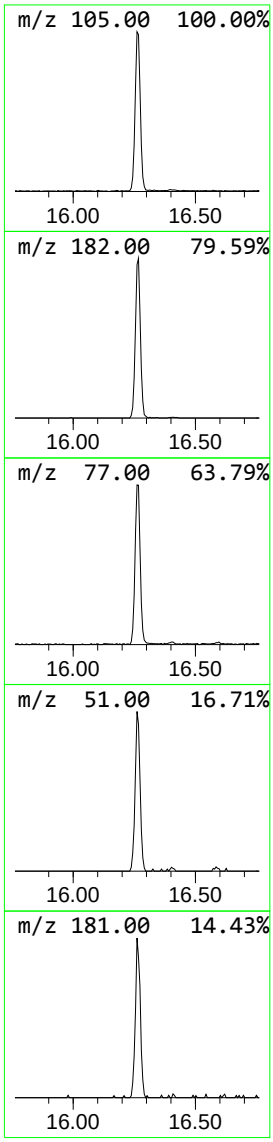
Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.261	15.51 ng	439685	Acenaphthene-d10	14.927

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Pyridine, 4,4'-(1,2-ethenediyl)bis-	182	C12H10N2	001135-32-6	47
3	.beta.-Carboline, 2-methyl-	182	C12H10N2	013099-99-5	46
4	2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	46
5	1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	43





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Data File : BG056306.D
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Sample : 01132-01
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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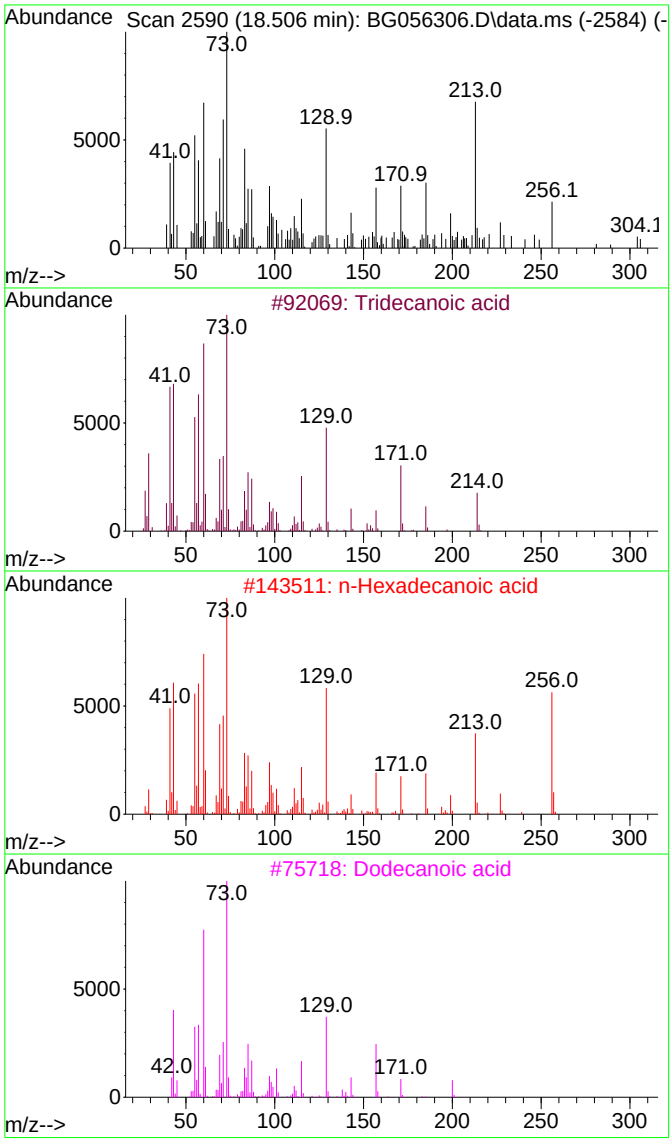
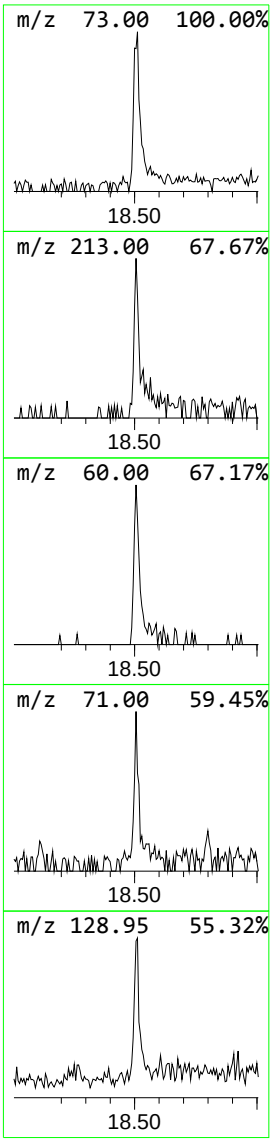
Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.506	2.57 ng	97269	Phenanthrene-d10	17.665

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	46
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	43





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Sample : 01132-01
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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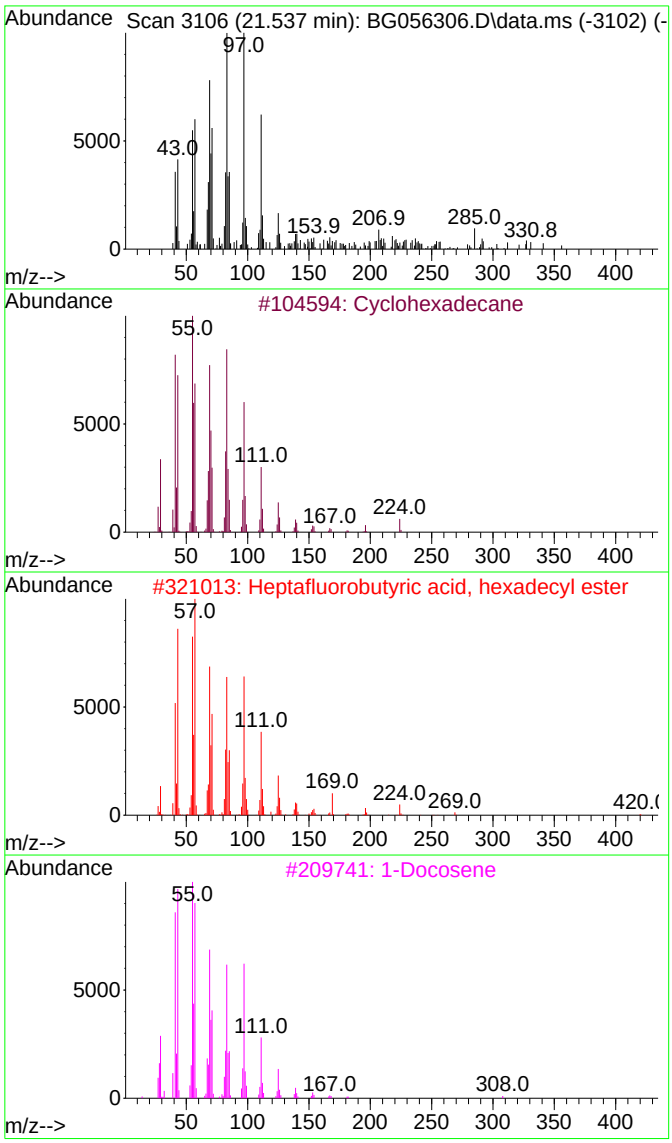
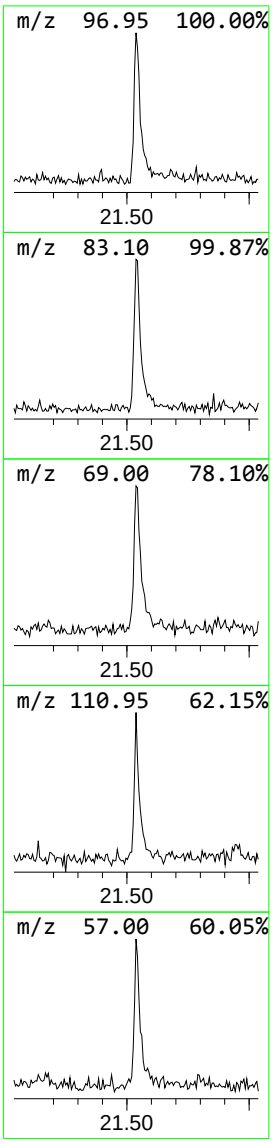
Peak Number 5 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.537	3.78 ng	150802	Chrysene-d12	21.954

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	86
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	68
3	1-Docosene	308	C22H44	001599-67-3	62
4	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	62
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	62





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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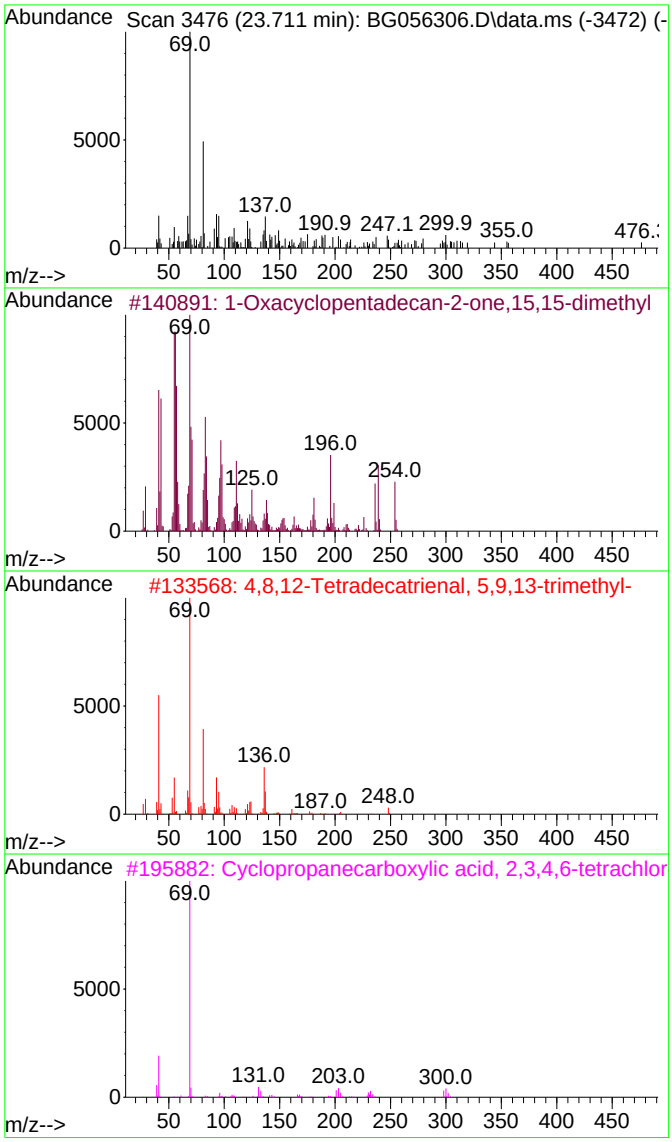
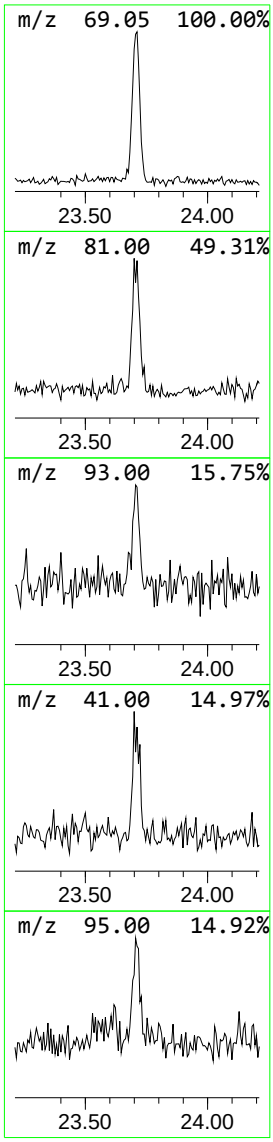
****
Peak Number 6 1-Oxacyclopentadecan-2-one,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.711	2.13 ng	90191	Perylene-d12	25.403

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Oxacyclopentadecan-2-one,15,15...	254	C16H30O2	1000196-63-1	62
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	62
3	Cyclopropanecarboxylic acid, 2,3...	298	C10H6Cl4O2	1000354-66-5	53
4	Supraene	410	C30H50	007683-64-9	52
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	52





Tentatively Identified Compound (LSC) summary

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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
unknown3.329	3.329	18.2	ng	226428	1	8.318	248591	20.0
2-Pentanone, 4-...	5.356	16.1	ng	200616	1	8.318	248591	20.0
Benzophenone	16.261	15.5	ng	439685	3	14.927	567109	20.0
Tridecanoic acid	18.506	2.6	ng	97269	4	17.665	756976	20.0
Cyclohexadecane	21.537	3.8	ng	150802	5	21.954	798356	20.0
1-Oxacyclopenta...	23.711	2.1	ng	90191	6	25.403	847846	20.0