LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011623\
Data File : BG056299.D
Acq On : 16 Jan 2023 16:46
Operator : CG/JU
Sample : 01133-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-2

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: BG056299.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.330	3	7	16	rVB	179246	253908	7.74%	1.822%
2	5.351	346	351	357	rBV	123627	188214	5.73%	1.351%
3	5.833	426	433	445	rVB	512842	816125	24.86%	5.856%
4	7.449	701	708	717	rBV	511620	860951	26.23%	6.178%
5	8.312	847	855	866	rVB	121247	208602	6.36%	1.497%
6	9.488	1048	1055	1063	rBV	296464	525341	16.00%	3.770%
7	11.144	1330	1337	1347	rBV	157860	284040	8.65%	2.038%
8	13.553	1740	1747	1756	rBV	1106682	1675578	51.05%	12.024%
9	14.928	1973	1981	1990	rBV	293962	466273	14.21%	3.346%
10	16.262	2202	2208	2216	rBV	173095	257705	7.85%	1.849%
11	16.403	2226	2232	2242	rBV	833889	1270181	38.70%	9.115%
12	17.660	2438	2446	2453	rBV	432762	664447	20.24%	4.768%
13	18.506	2584	2590	2599	rBV2	75243	116341	3.54%	0.835%
14	19.764	2800	2804	2809	rBV2	33965	41894	1.28%	0.301%
15	20.240	2879	2885	2891	rVB	2499769	3282438	100.00%	23.554%
16	21.544	3102	3107	3111	rBV5	33079	52241	1.59%	0.375%
17	21.838	3154	3157	3165	rVB2	28176	51228	1.56%	0.368%
18	21.955	3170	3177	3190	rVB2	473313	807243	24.59%	5.793%
19	23.166	3380	3383	3389	rVB8	18537	36235	1.10%	0.260%
20	23.706	3469	3475	3482	rVB2	51279	103529	3.15%	0.743%
21	25.398	3752	3763	3775	rVB2	276211	839178	25.57%	6.022%
22	29.411	4423	4446	4461	rBV3	123408	844270	25.72%	6.058%
23	30.586	4633	4646	4647	rBV5	116581	289696	8.83%	2.079%

Sum of corrected areas: 13935658

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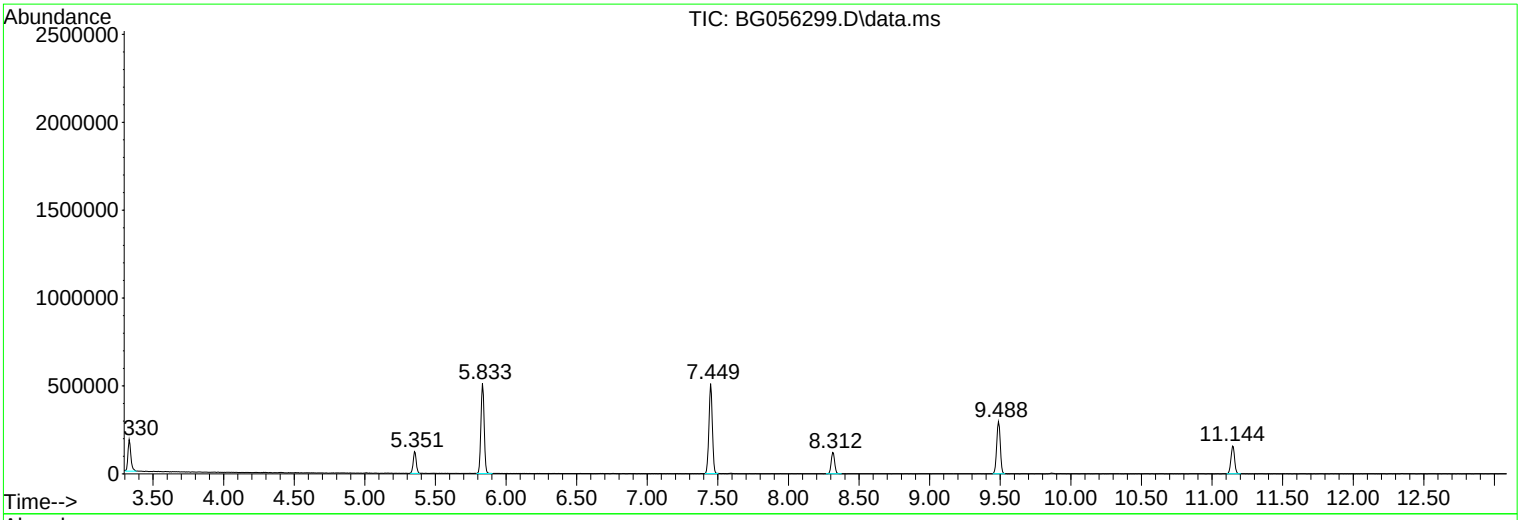
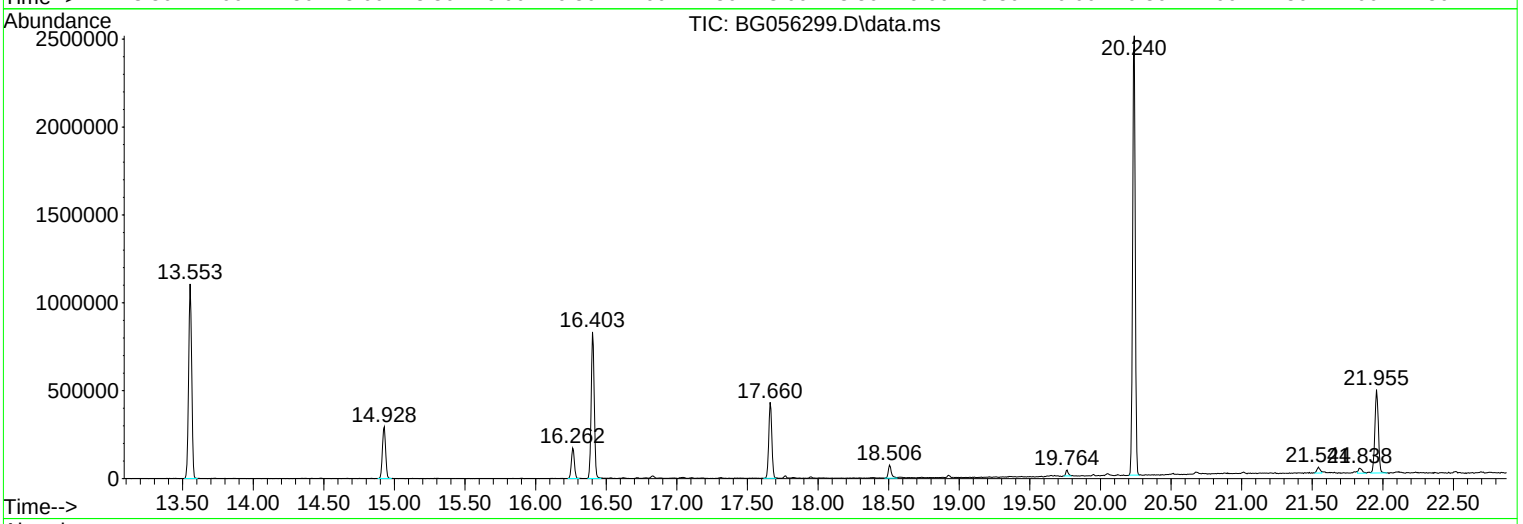
Misc :
ALS Vial : 9 Sample Multiplier: 1

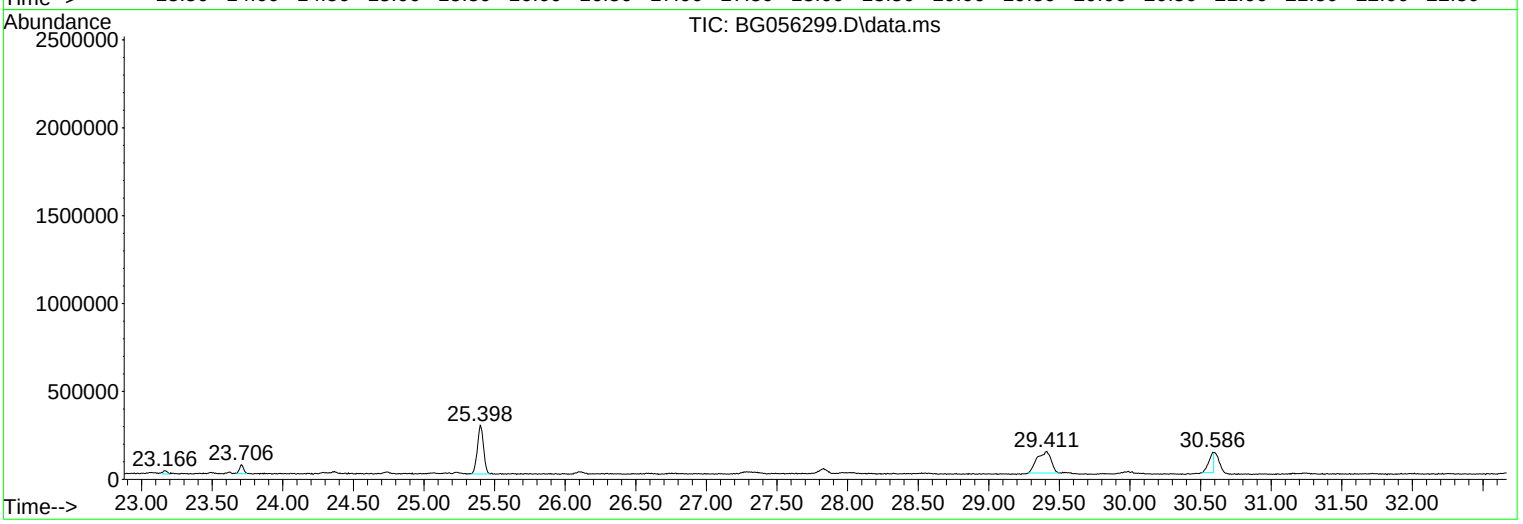
Instrument :
BNA_G
ClientSampleId :
COMPOSITE-2

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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Operator : CG/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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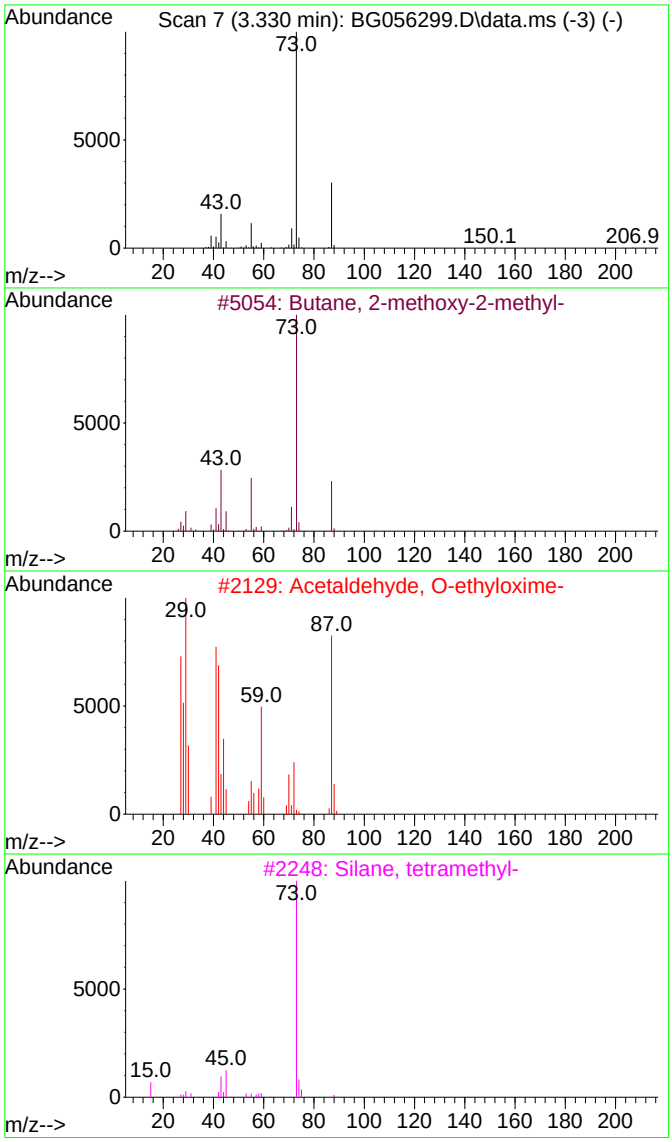
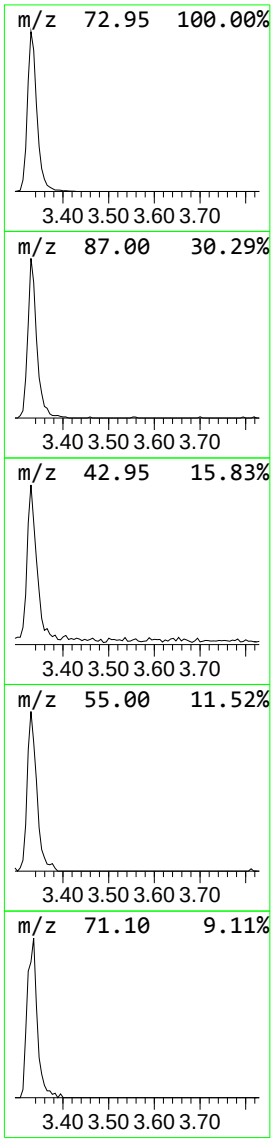
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.330	24.34 ng	253908	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	64
2	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7





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Acq On : 16 Jan 2023 16:46
Operator : CG/JU
Sample : 01133-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-2

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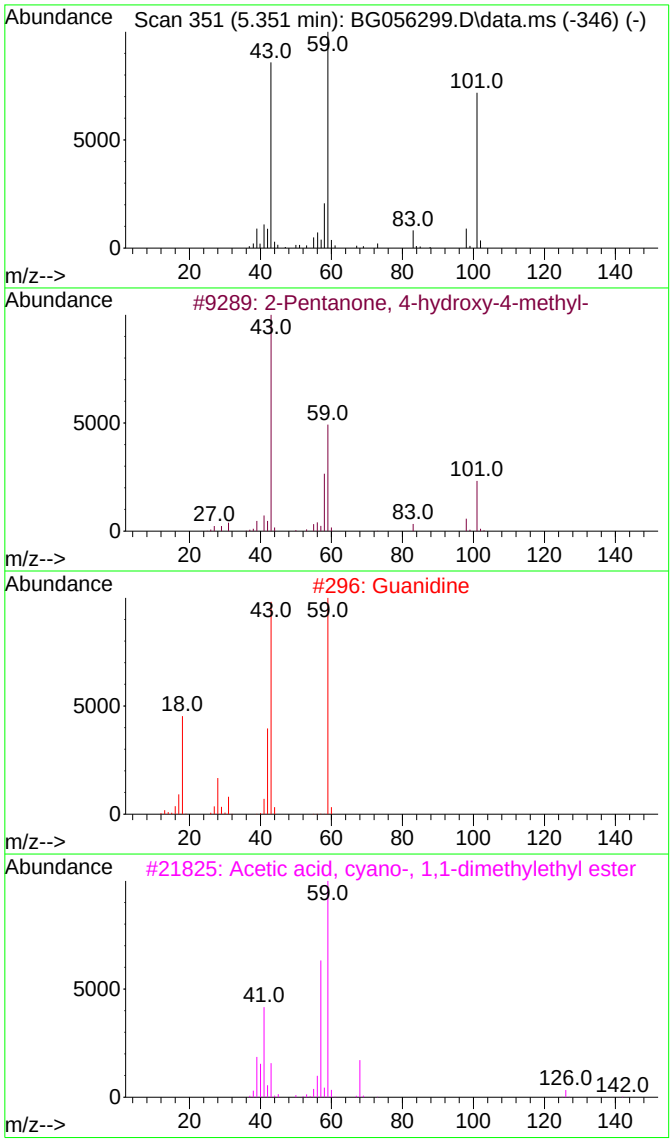
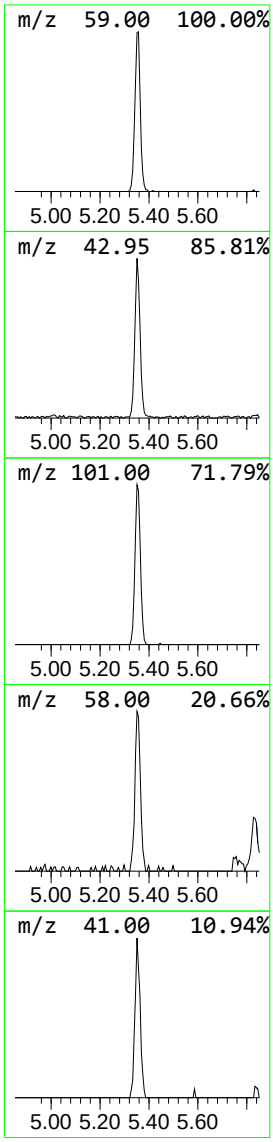
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.351	18.05 ng	188214	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25





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Operator : CG/JU
Sample : 01133-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-2

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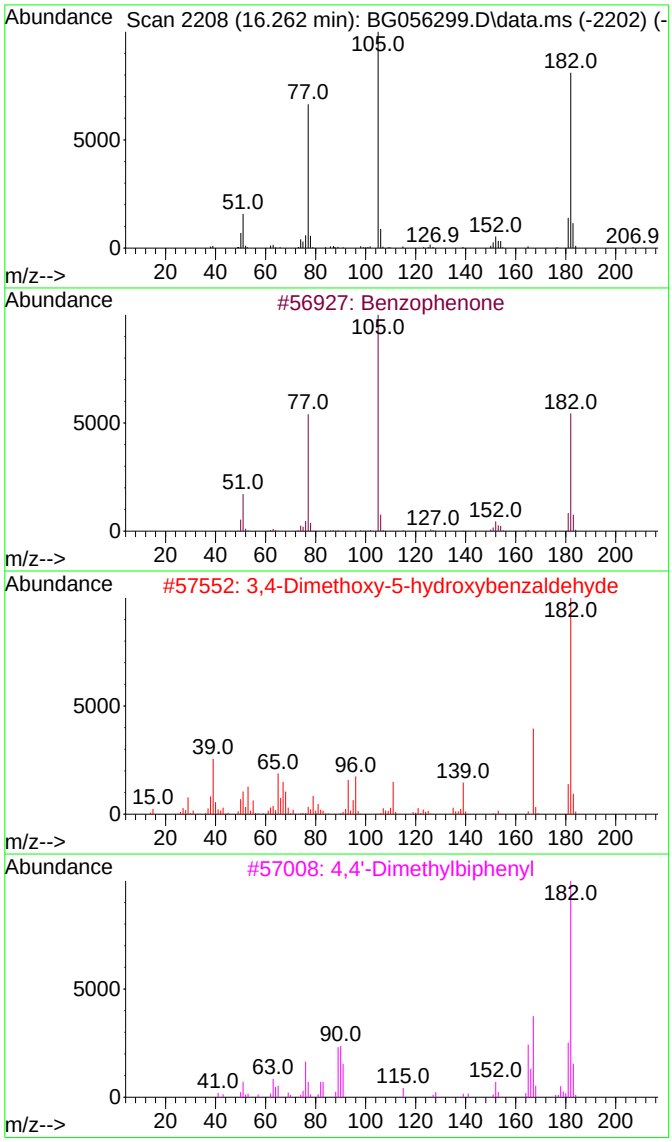
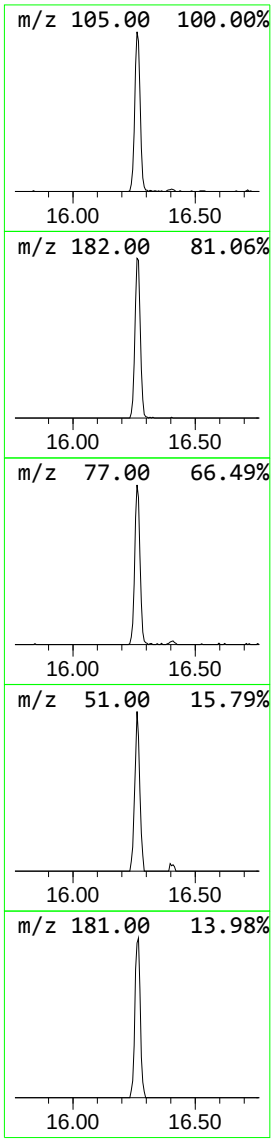
Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.262	11.05 ng	257705	Acenaphthene-d10	14.928

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	3,4-Dimethoxy-5-hydroxybenzaldehyde	182	C9H10O4	029865-90-5	47
3	4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	46
4	1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	46
5	1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	43





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Operator : CG/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-2

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
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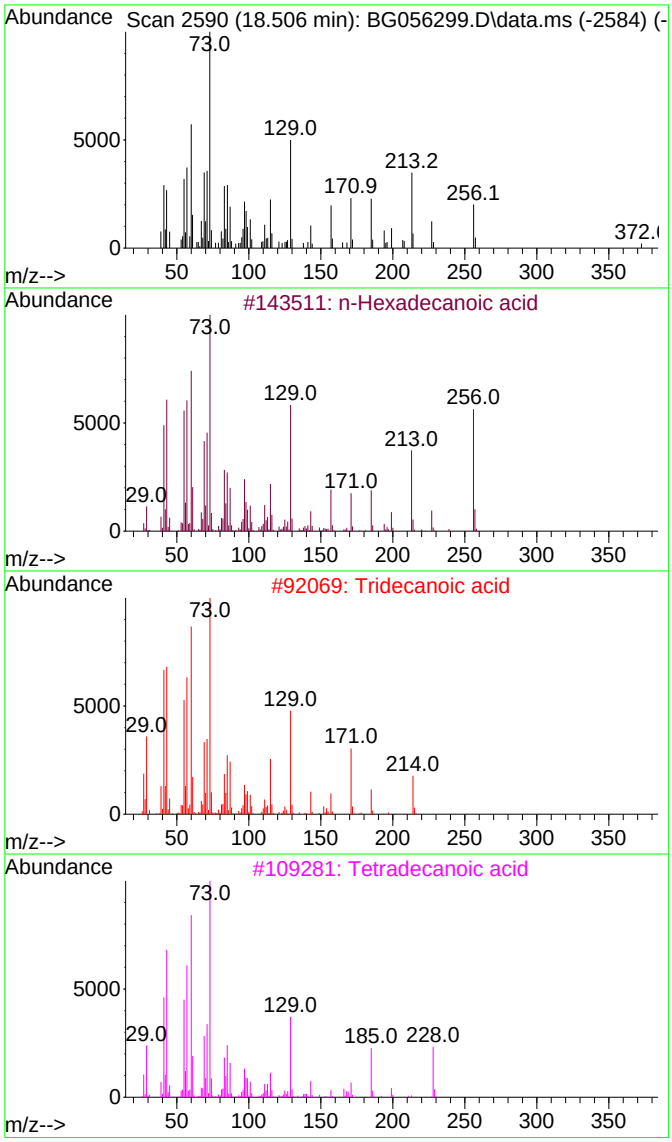
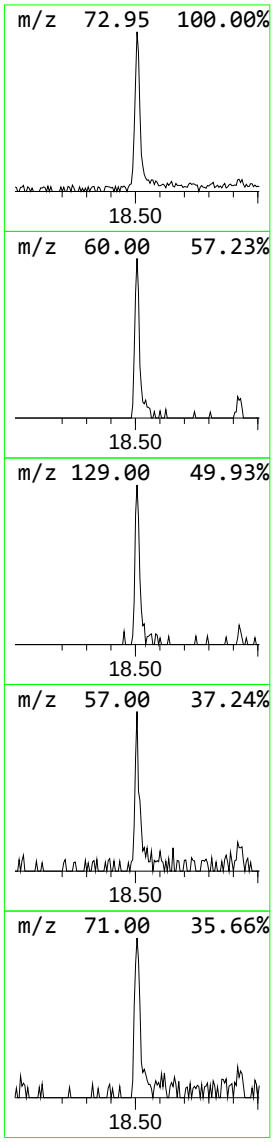
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.506	3.50 ng	116341	Phenanthrene-d10	17.660

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	92
4	Octadecanoic acid	284	C18H36O2	000057-11-4	49
5	Dodecanoic acid	200	C12H24O2	000143-07-7	35





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Sample : 01133-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMPOSITE-2

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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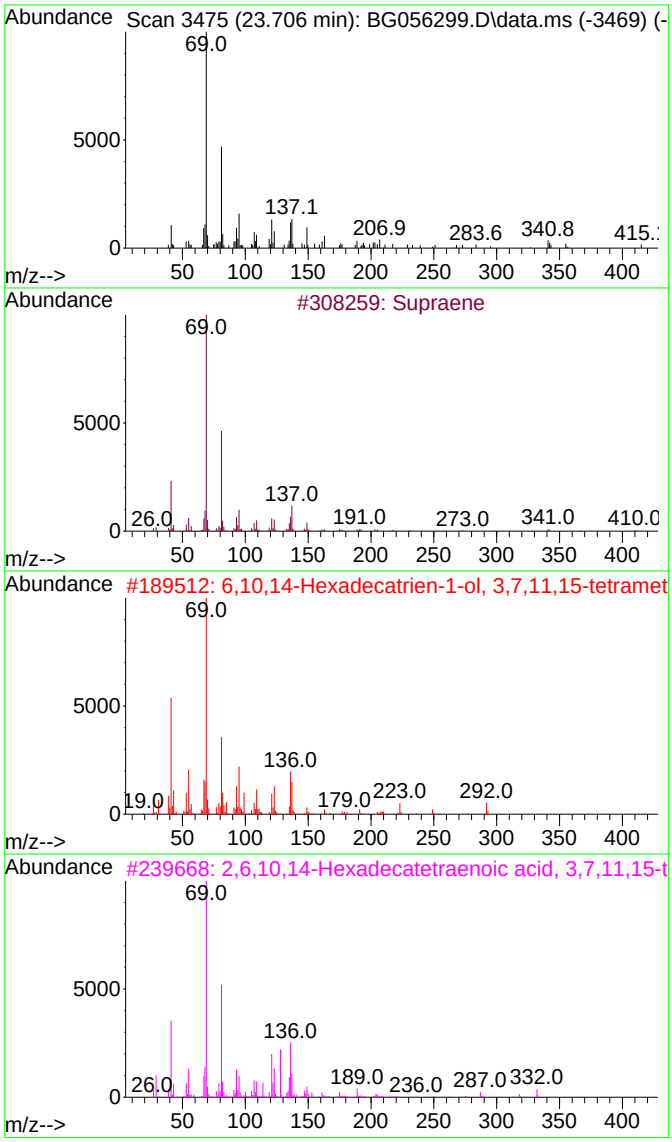
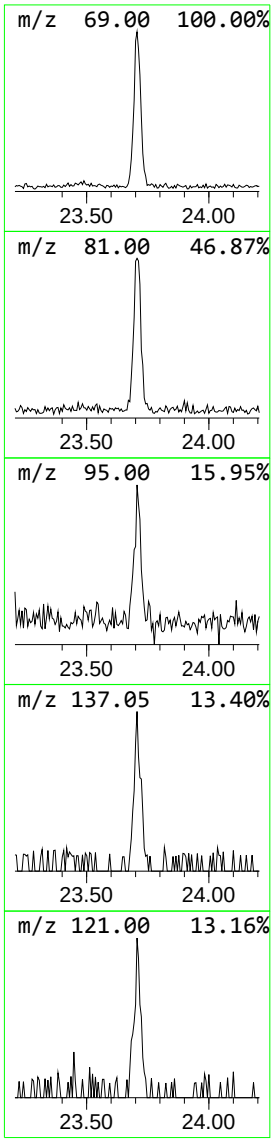
Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.706	2.47 ng	103529	Perylene-d12	25.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	64
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	55
5	3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	53





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.330	24.3	ng	253908	1	8.318	208602	20.0
2-Pentanone, 4-...	5.351	18.1	ng	188214	1	8.318	208602	20.0
Benzophenone	16.262	11.1	ng	257705	3	14.928	466273	20.0
n-Hexadecanoic ...	18.506	3.5	ng	116341	4	17.660	664447	20.0
Supraene	23.706	2.5	ng	103529	6	25.398	839178	20.0