LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057827.D
Acq On : 23 Jun 2023 3:55
Operator : CG/JU
Sample : 03320-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-14

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: BG057827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.029	324	330	339	rBV	487471	711877	28.54%	4.273%
2	5.493	402	409	420	rBV	949029	1450271	58.14%	8.705%
3	6.104	506	513	522	rBV2	20017	32135	1.29%	0.193%
4	7.086	671	680	689	rBV	919306	1562766	62.65%	9.380%
5	7.920	816	822	829	rBV	189926	309006	12.39%	1.855%
6	9.083	1010	1020	1030	rBV	555522	959494	38.46%	5.759%
7	10.723	1287	1299	1309	rBV	265784	469945	18.84%	2.821%
8	13.178	1710	1717	1725	rBV	1264655	1944378	77.95%	11.670%
9	14.553	1945	1951	1962	rVB	386984	607929	24.37%	3.649%
10	15.911	2176	2182	2187	rBV	142968	191066	7.66%	1.147%
11	16.040	2197	2204	2216	rBV	1039493	1568694	62.89%	9.415%
12	16.692	2310	2315	2322	rBV2	19049	28796	1.15%	0.173%
13	17.297	2412	2418	2424	rBV	476883	701495	28.12%	4.210%
14	17.468	2442	2447	2458	rBV4	15029	36201	1.45%	0.217%
15	18.061	2543	2548	2555	rBV4	26533	48443	1.94%	0.291%
16	18.190	2564	2570	2584	rBV	266304	416682	16.70%	2.501%
17	19.348	2759	2767	2773	rBV2	43544	89135	3.57%	0.535%
18	19.459	2782	2786	2797	rBV2	58874	102300	4.10%	0.614%
19	19.712	2822	2829	2834	rVB2	18123	36405	1.46%	0.219%
20	19.918	2858	2864	2869	rBV	1853328	2494511	100.00%	14.972%
21	21.204	3079	3083	3091	rVV4	130916	208686	8.37%	1.253%
22	21.287	3093	3097	3104	rVB	53346	80445	3.22%	0.483%
23	21.551	3135	3142	3147	rBV2	440601	740892	29.70%	4.447%
24	22.109	3231	3237	3247	rVB	329725	551994	22.13%	3.313%
25	23.208	3418	3424	3434	rVB	287240	540232	21.66%	3.242%
26	24.706	3669	3679	3693	rBV2	239107	777322	31.16%	4.665%

Sum of corrected areas: 16661100

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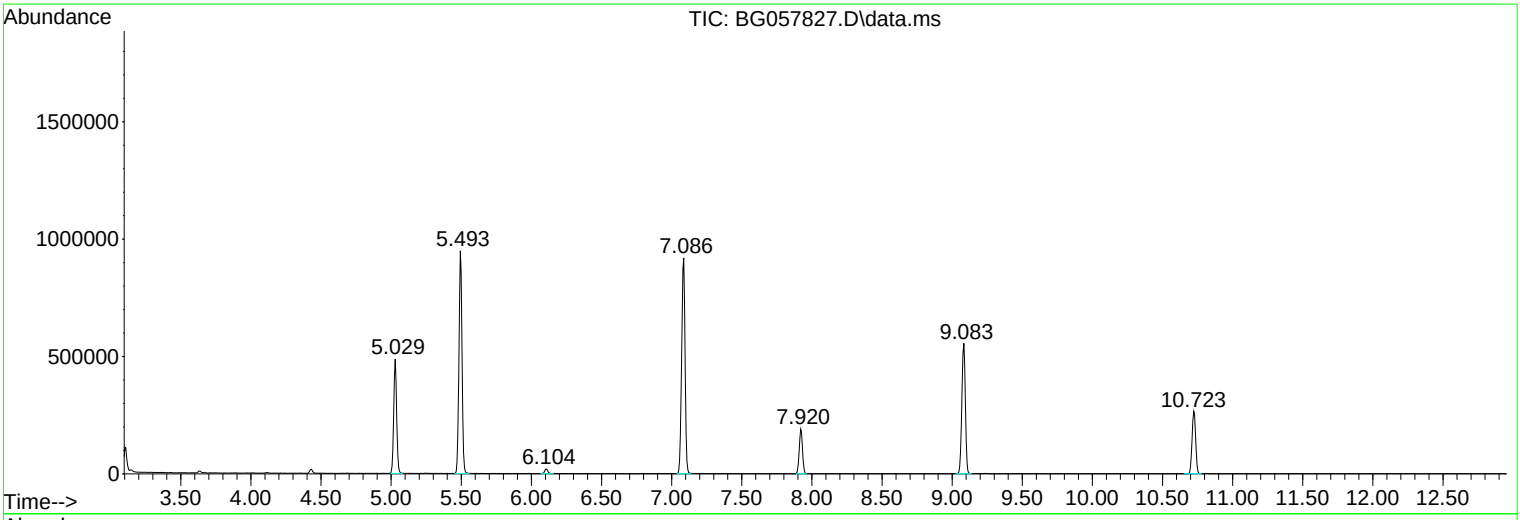
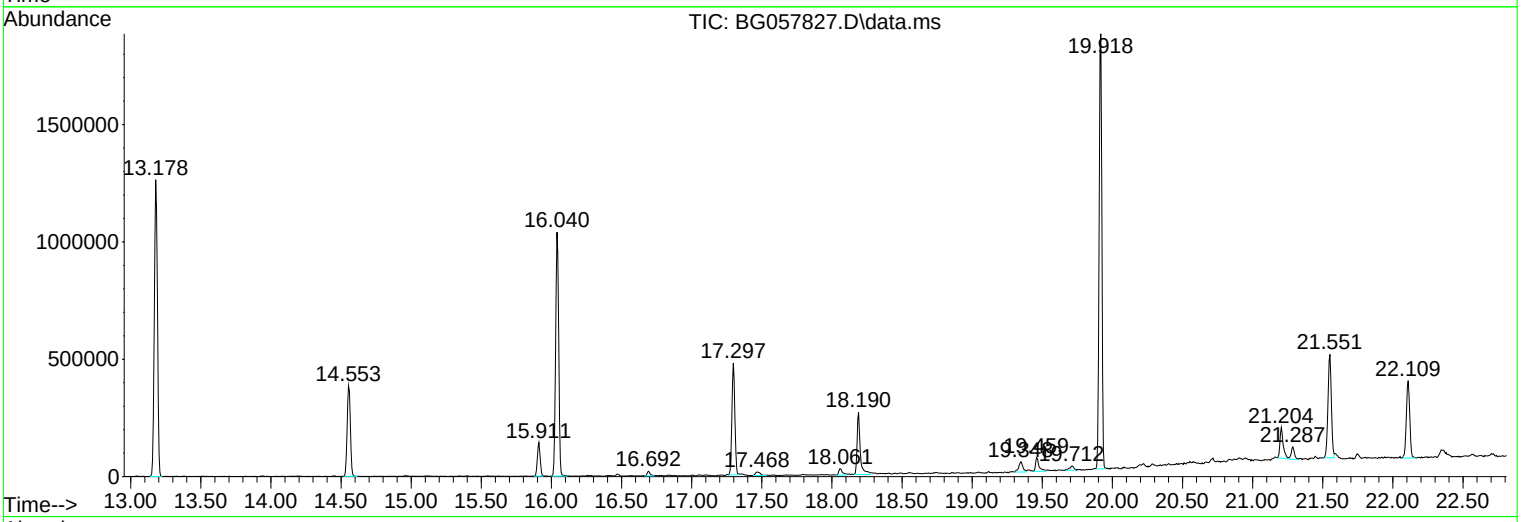
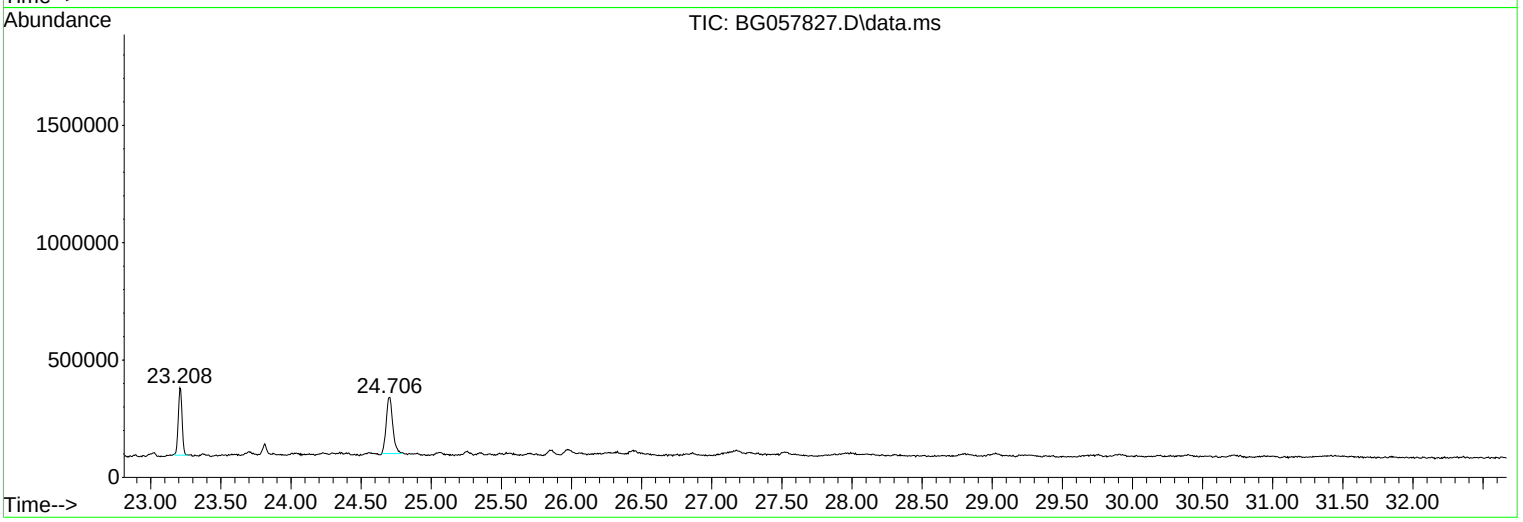
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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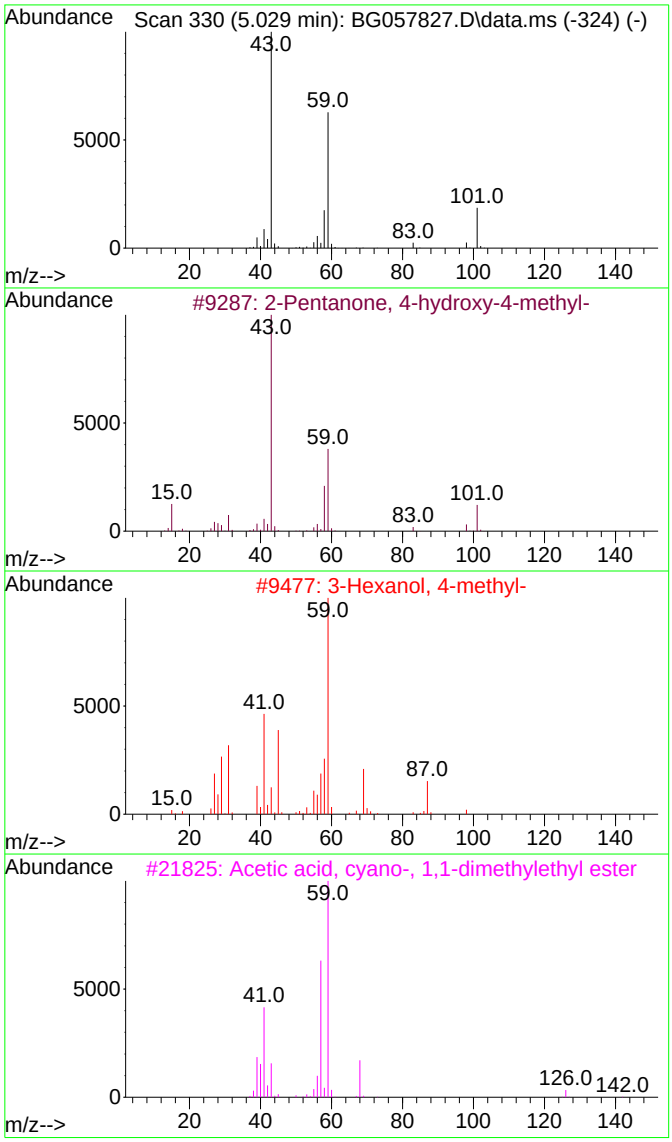
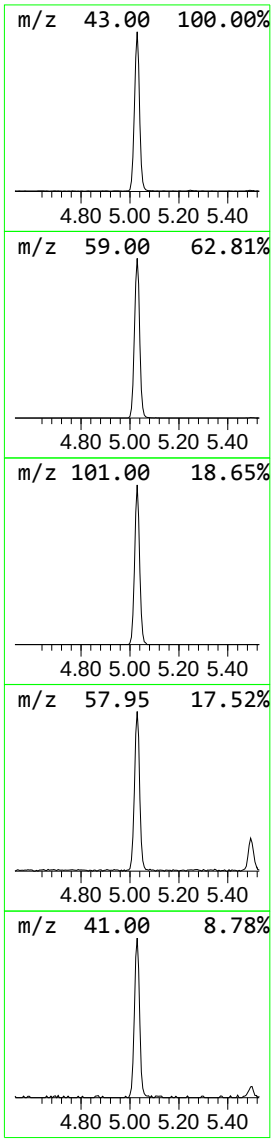
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.029	46.08 ng	711877	1,4-Dichlorobenzene-d4	7.920

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Operator : CG/JU
Sample : 03320-13
Misc :
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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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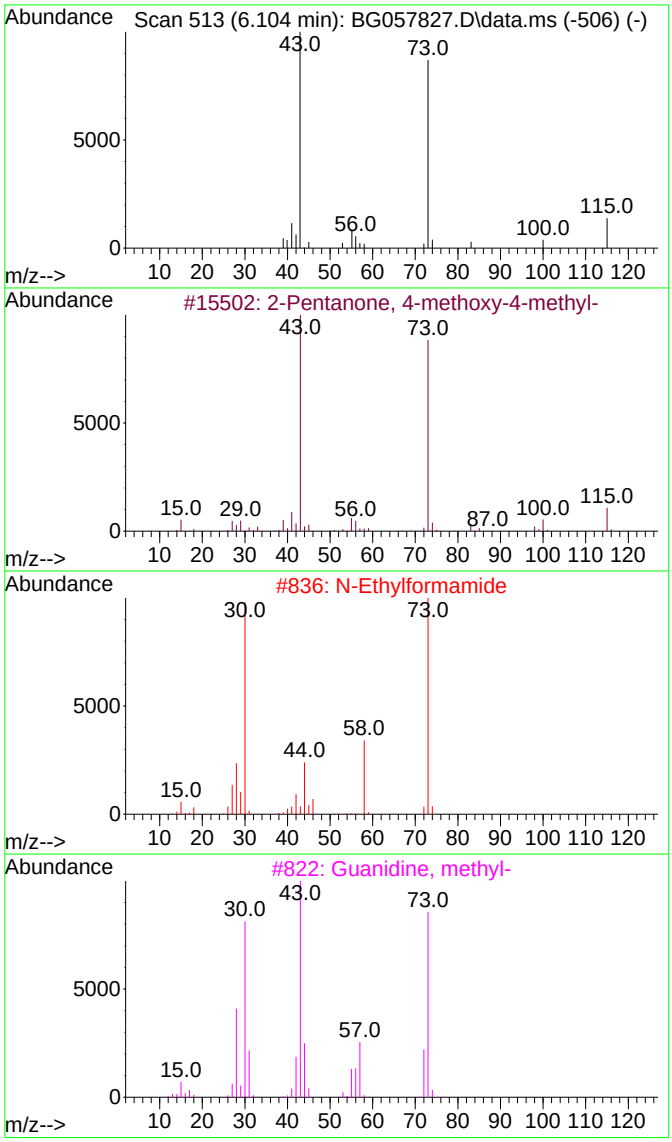
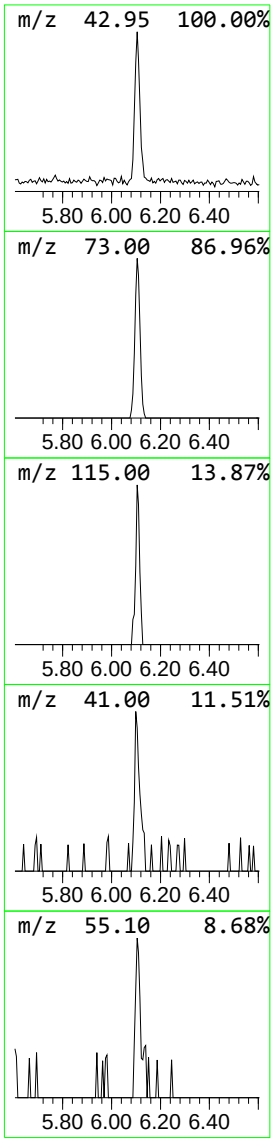
****
Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.104	2.08 ng	32135	1,4-Dichlorobenzene-d4	7.920

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2	N-Ethylformamide	73	C3H7NO	000627-45-2	16
3	Guanidine, methyl-	73	C2H7N3	000471-29-4	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9





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Operator : CG/JU
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
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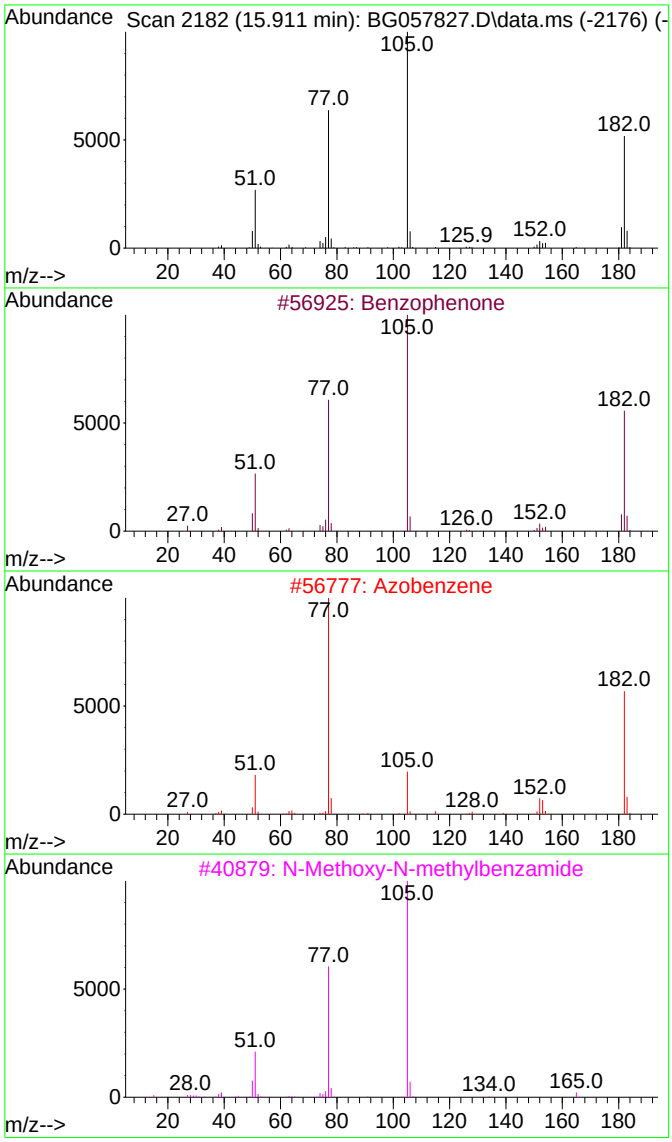
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

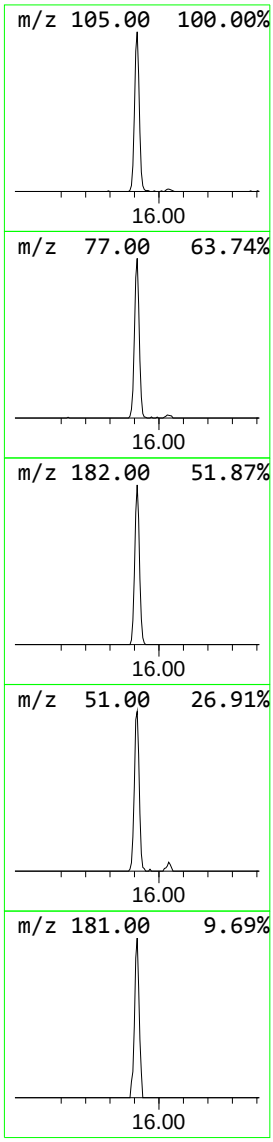
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.911	6.29 ng	191066	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	53
3	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5	Benzoyl bromide	184	C7H5BrO	000618-32-6	47





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-14

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

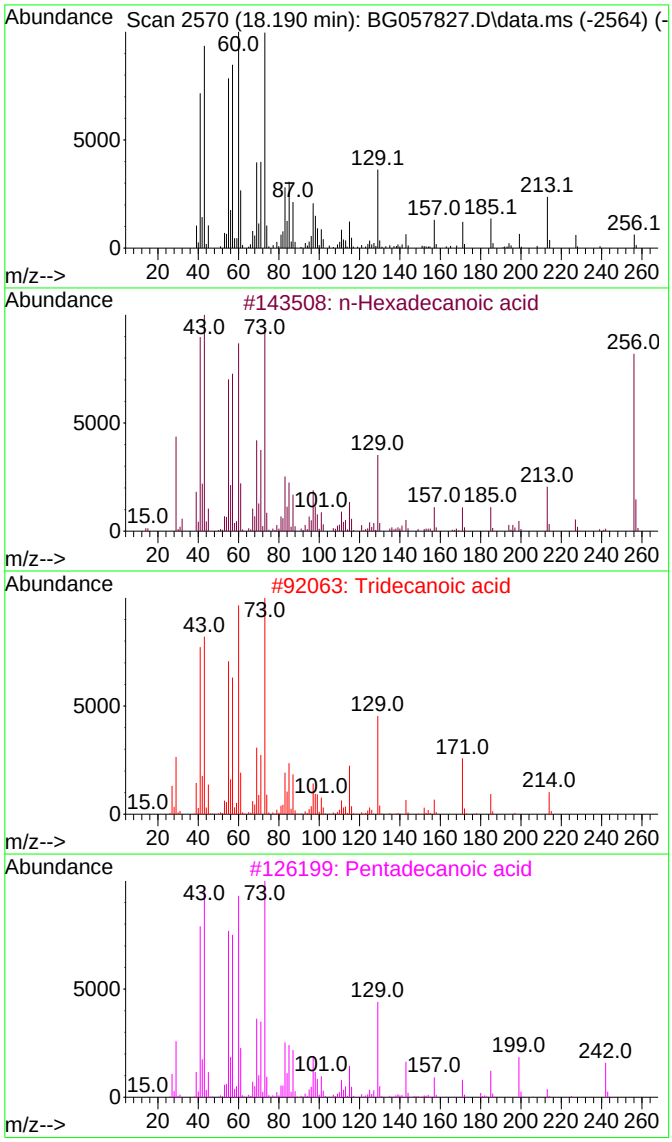
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

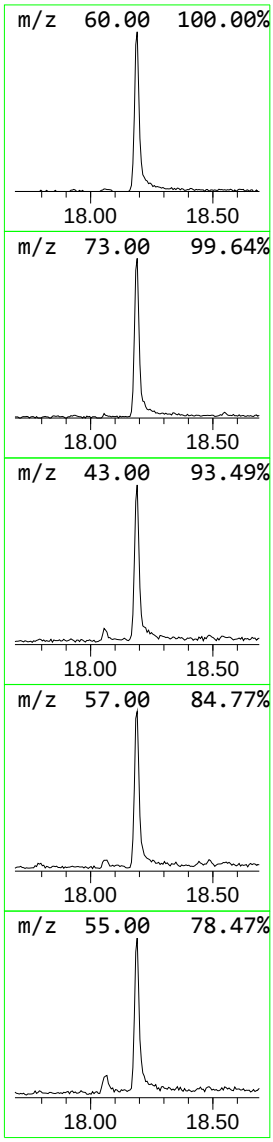
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.190	11.88 ng	416682	Phenanthrene-d10	17.297

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057827.D
Acq On : 23 Jun 2023 3:55
Operator : CG/JU
Sample : 03320-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
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TIC Library : C:\Database\NIST20.L
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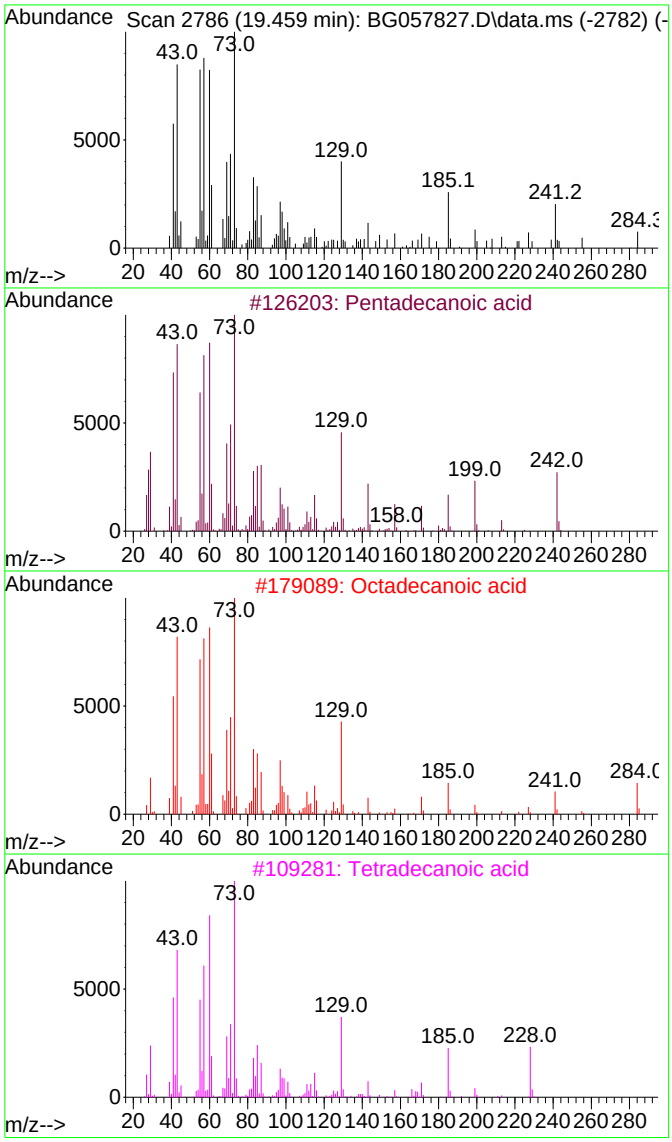
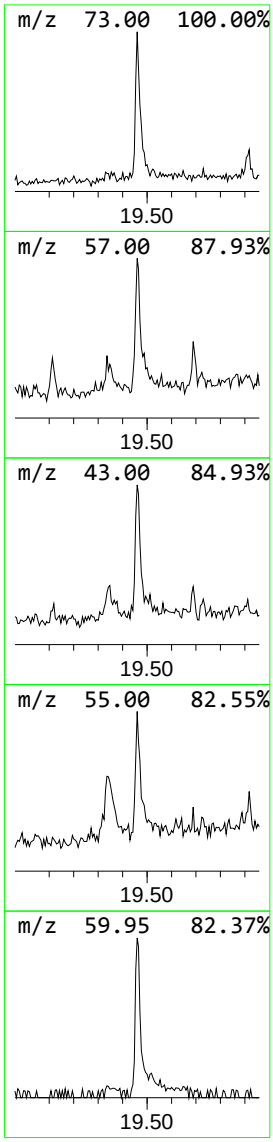
****

Peak Number 6 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.459	2.76 ng	102300	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Undecanoic acid	186	C11H22O2	000112-37-8	46
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30





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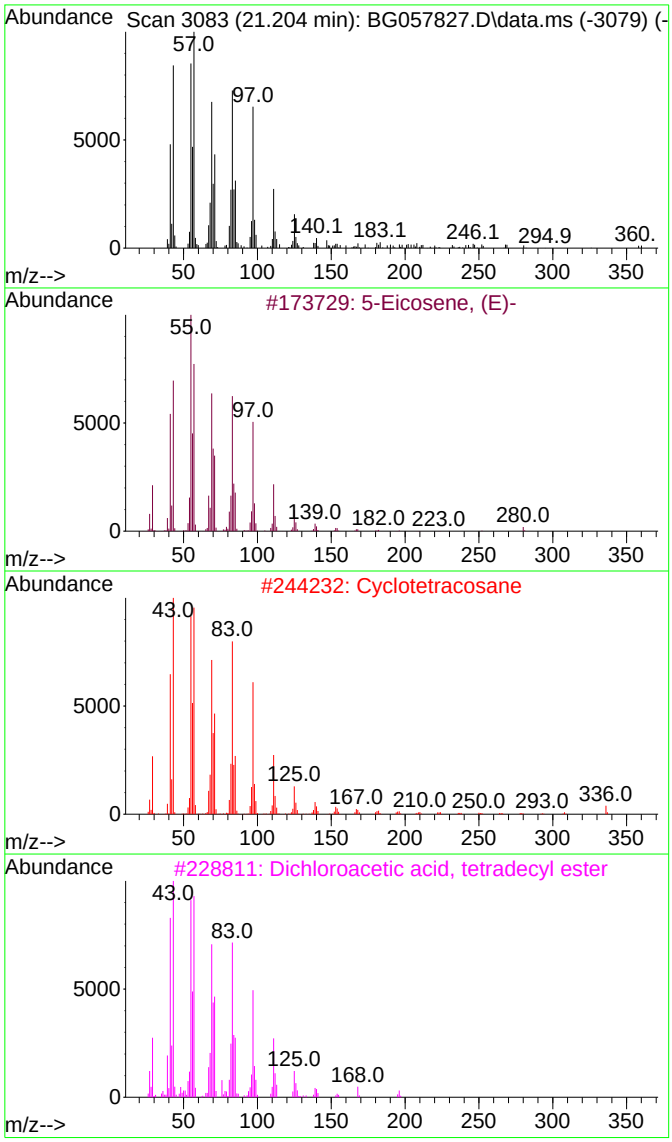
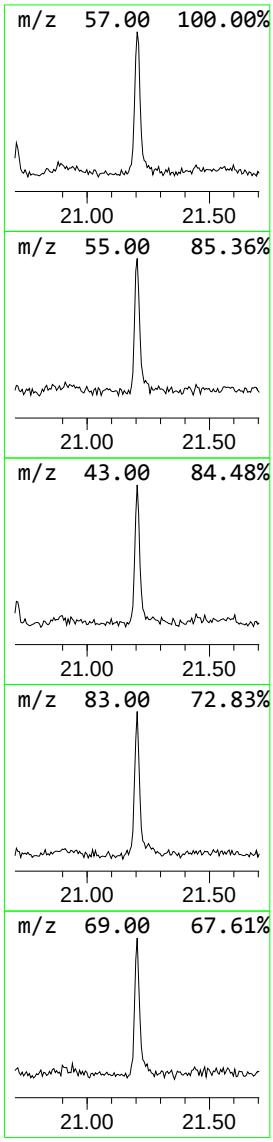
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.204	5.63 ng	208686	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Cyclotetracosane	336	C24H48	000297-03-0	91
3	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	91
4	1-Octadecene	252	C18H36	000112-88-9	90
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90





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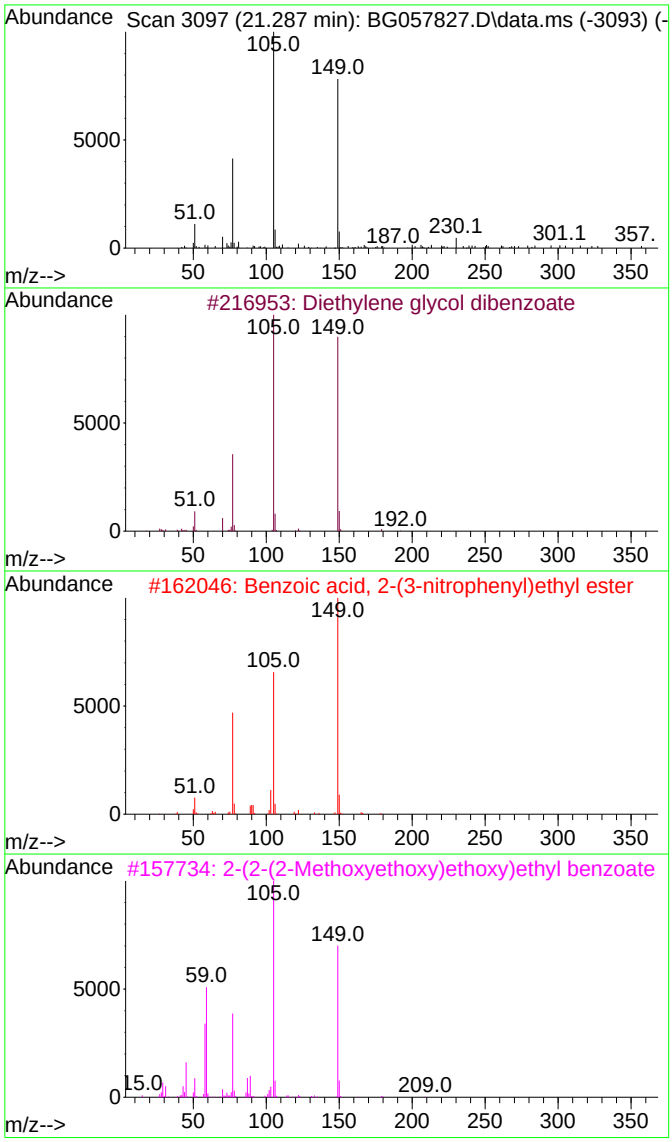
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

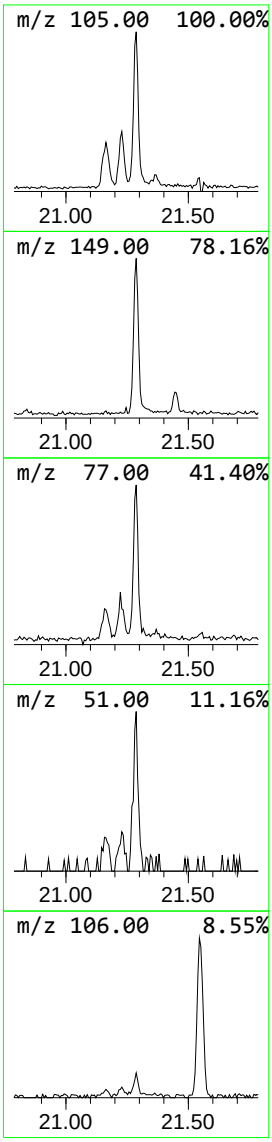
****

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.287	2.17 ng	80445	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
3	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	72
4	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
5	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	56





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TIC Library : C:\Database\NIST20.L
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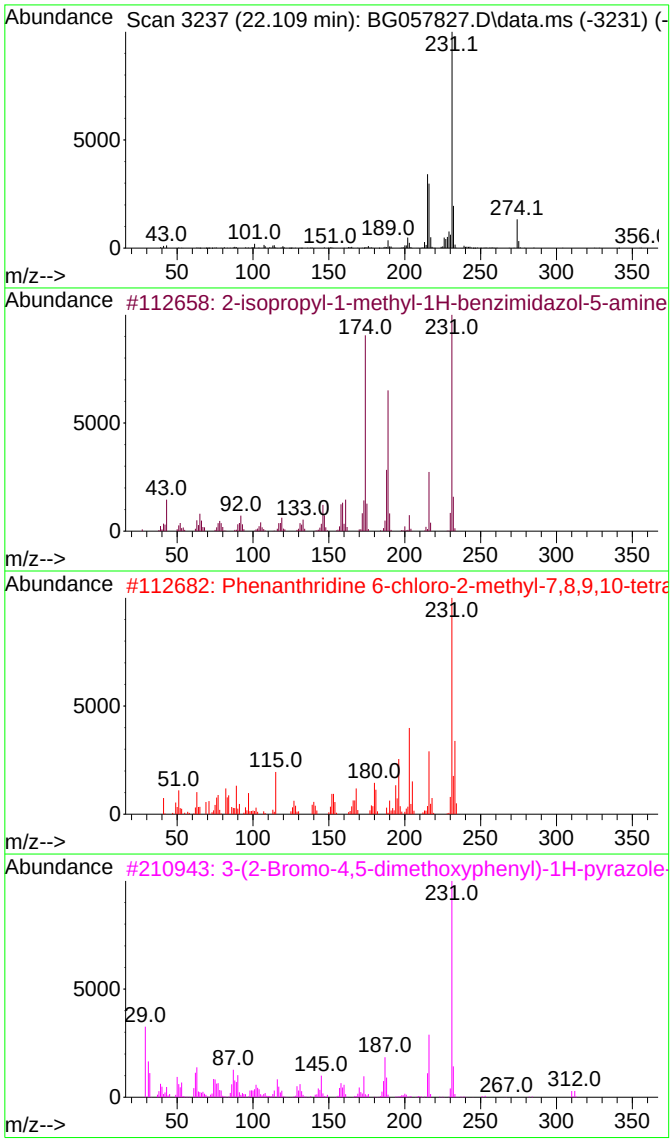
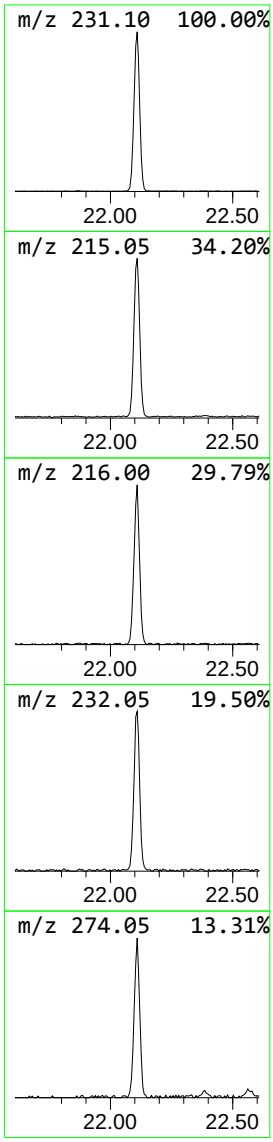
****
Peak Number 9 2-isopropyl-1-methyl-1H-ben... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.109	14.90 ng	551994	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-isopropyl-1-methyl-1H-benzimid...	231	C13H17N3O	1790918-16-9	53
2	Phenanthridine 6-chloro-2-methyl...	231	C14H14ClN	035417-77-7	53
3	3-(2-Bromo-4,5-dimethoxyphenyl)-...	310	C12H11BrN2O3	1000459-09-2	50
4	2-[(Methylamino)methylene]thiazo...	231	C11H9N3OS	072740-41-1	49
5	2-Benzothiazolamine, N-(1-methyl...	231	C12H13N3S	084859-07-4	47





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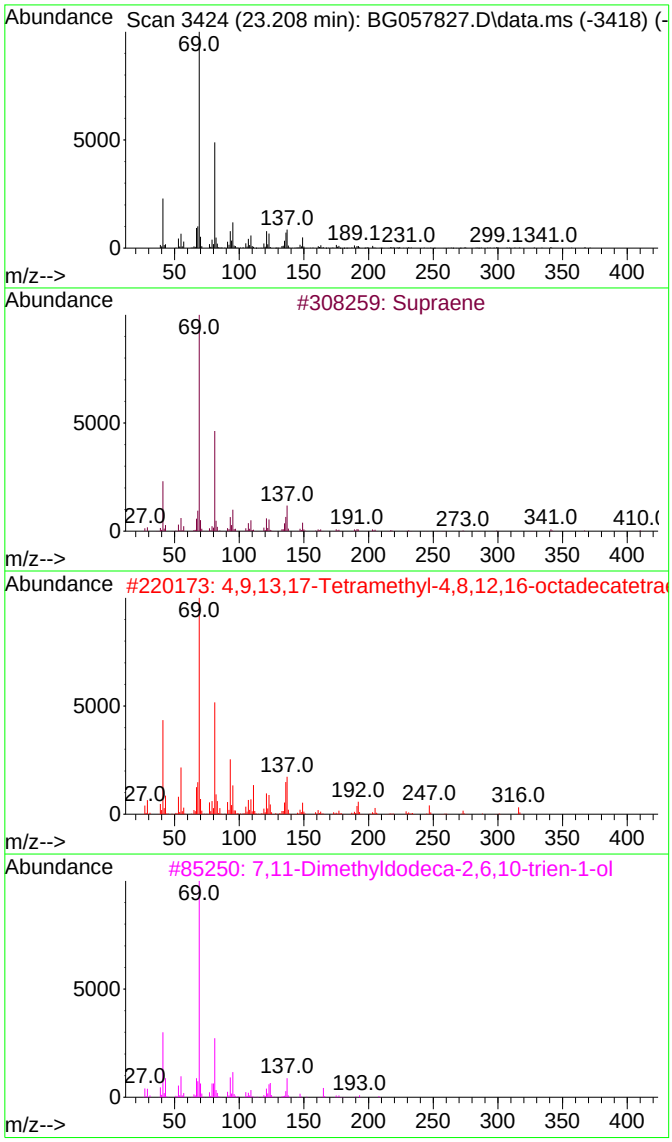
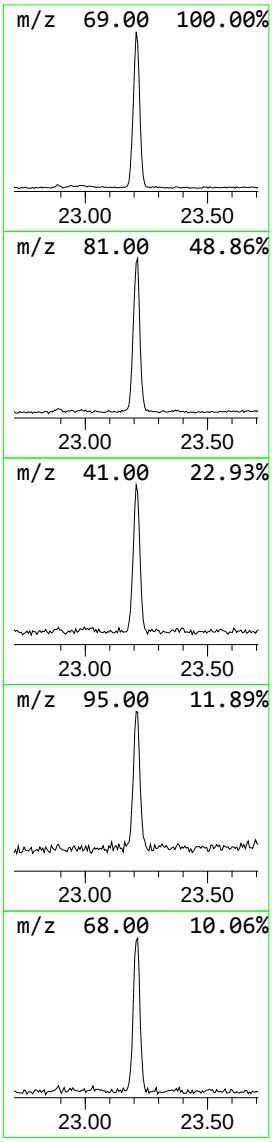
****

Peak Number 10 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.208	13.90 ng	540232	Perylene-d12	24.700

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	78
4	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	78
5	Farnesol isomer a	222	C15H26O	1000108-92-4	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057827.D
Acq On : 23 Jun 2023 3:55
Operator : CG/JU
Sample : 03320-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-14

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
2-Pentanone, 4-...	5.029	46.1	ng	711877	1	7.920	309006	20.0
2-Pentanone, 4-...	6.104	2.1	ng	32135	1	7.920	309006	20.0
Benzophenone	15.911	6.3	ng	191066	3	14.553	607929	20.0
n-Hexadecanoic ...	18.190	11.9	ng	416682	4	17.297	701495	20.0
Pentadecanoic acid	19.459	2.8	ng	102300	5	21.551	740892	20.0
5-Eicosene, (E)-	21.204	5.6	ng	208686	5	21.551	740892	20.0
Diethylene glyc...	21.287	2.2	ng	80445	5	21.551	740892	20.0
2-isopropyl-1-m...	22.109	14.9	ng	551994	5	21.551	740892	20.0
Supraene	23.208	13.9	ng	540232	6	24.700	777322	20.0