LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
Data File : BG056018.D
Acq On : 19 Dec 2022 18:08
Operator : CG/JU
Sample : N6089-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-24

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056018.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.400	14	19	30	rVB2	11713	20194	1.68%	0.445%
2	5.415	356	362	368	rBB	26788	40354	3.36%	0.888%
3	5.891	436	443	450	rBB	198445	313323	26.05%	6.898%
4	7.501	709	717	724	rBB	193354	333501	27.73%	7.342%
5	8.370	859	865	871	rBB	32760	52691	4.38%	1.160%
6	9.539	1057	1064	1071	rBB	120632	210521	17.50%	4.635%
7	11.202	1340	1347	1354	rBB	41100	70560	5.87%	1.553%
8	13.605	1749	1756	1763	rBB	411338	629831	52.37%	13.866%
9	14.974	1983	1989	1995	rBB	76649	114823	9.55%	2.528%
10	16.314	2212	2217	2222	rBV2	15248	21351	1.78%	0.470%
11	16.449	2234	2240	2253	rBB	436412	677928	56.37%	14.924%
12	17.712	2448	2455	2460	rBV	109083	164747	13.70%	3.627%
13	18.558	2594	2599	2606	rBV3	33087	44270	3.68%	0.975%
14	19.810	2806	2812	2820	rVV5	10206	14361	1.19%	0.316%
15	20.098	2857	2861	2867	rVB	14286	19947	1.66%	0.439%
16	20.286	2887	2893	2899	rBV	937446	1202669	100.00%	26.477%
17	21.602	3113	3117	3126	rVB2	26436	38997	3.24%	0.859%
18	22.019	3180	3188	3193	rBV	116506	217510	18.09%	4.788%
19	24.939	3678	3685	3695	rBV9	8602	23798	1.98%	0.524%
20	25.180	3720	3726	3733	rBV2	4948	13818	1.15%	0.304%
21	25.327	3746	3751	3762	rBV3	5581	14534	1.21%	0.320%
22	25.515	3772	3783	3795	rBV2	69352	218663	18.18%	4.814%
23	26.379	3923	3930	3931	rBV5	8452	14316	1.19%	0.315%
24	28.159	4225	4233	4235	rBV7	10164	20885	1.74%	0.460%
25	30.444	4607	4622	4626	rBV9	12098	48795	4.06%	1.074%

Sum of corrected areas: 4542387

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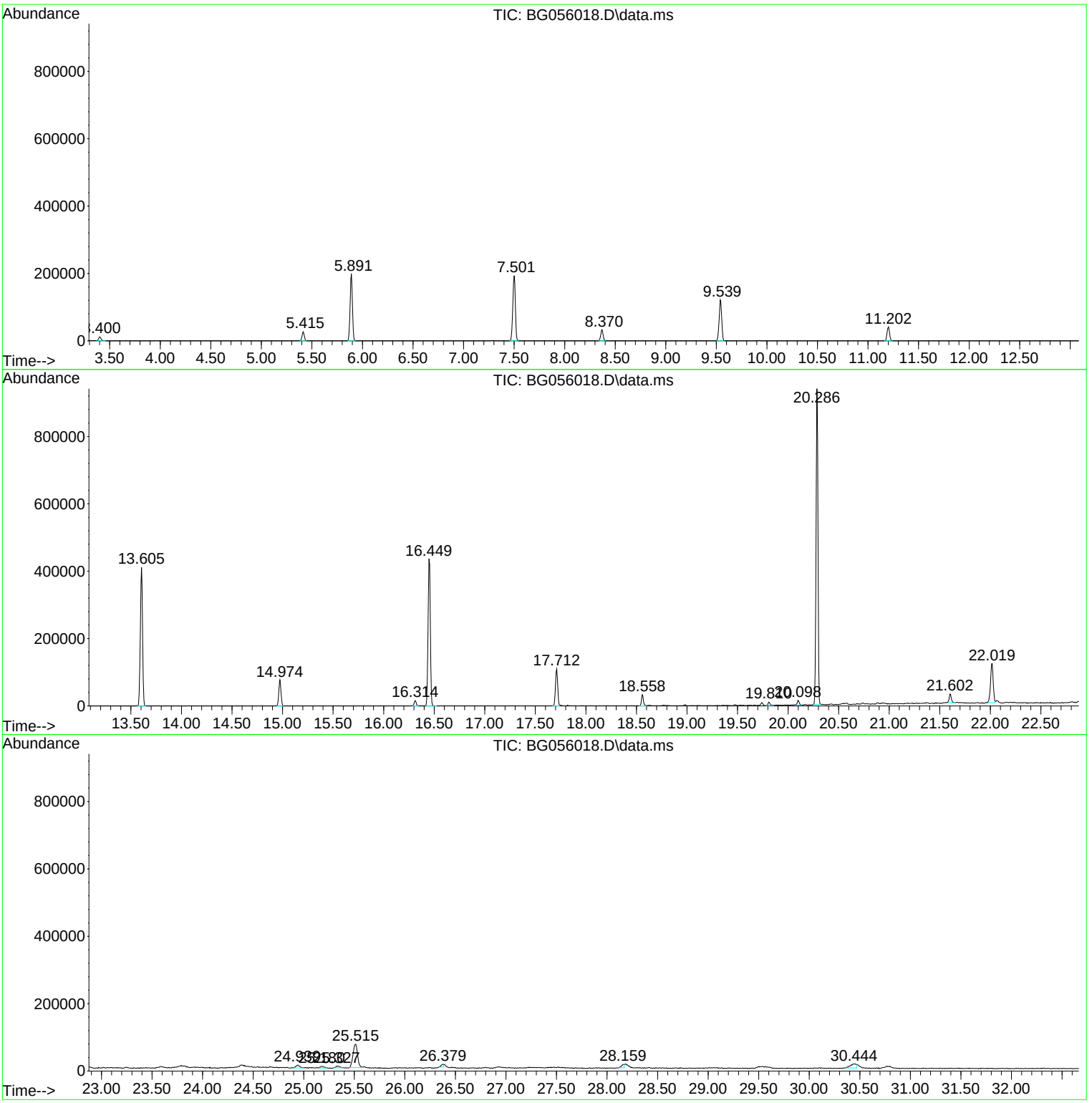
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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\BG121922\
Data File : BG056018.D
Acq On : 19 Dec 2022 18:08
Operator : CG/JU
Sample : N6089-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

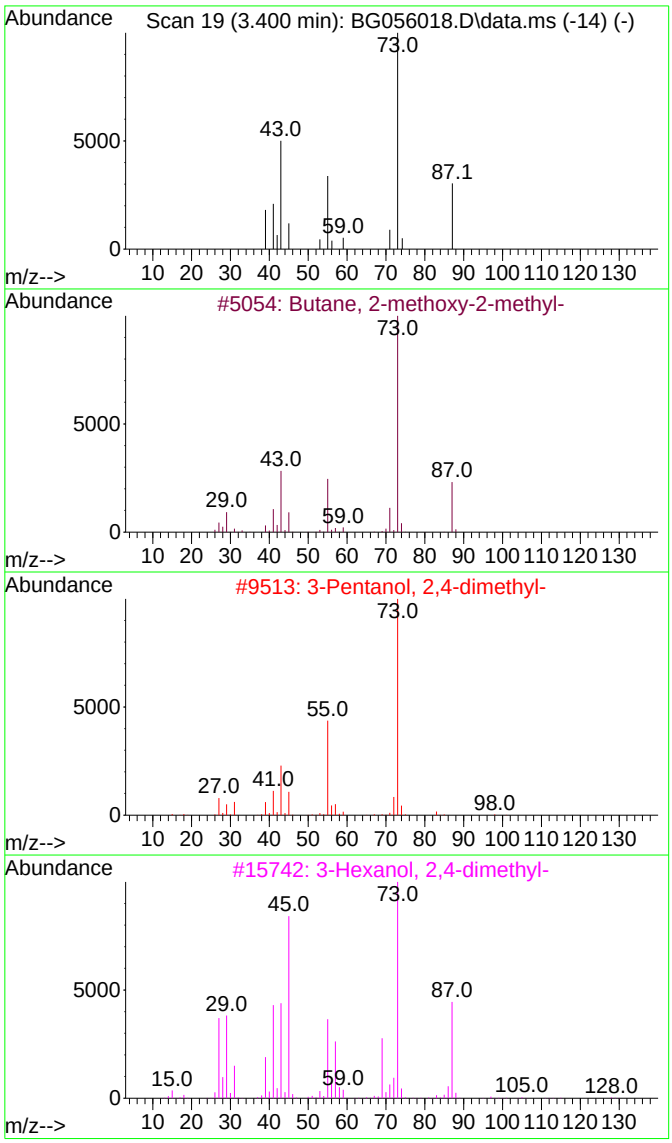
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

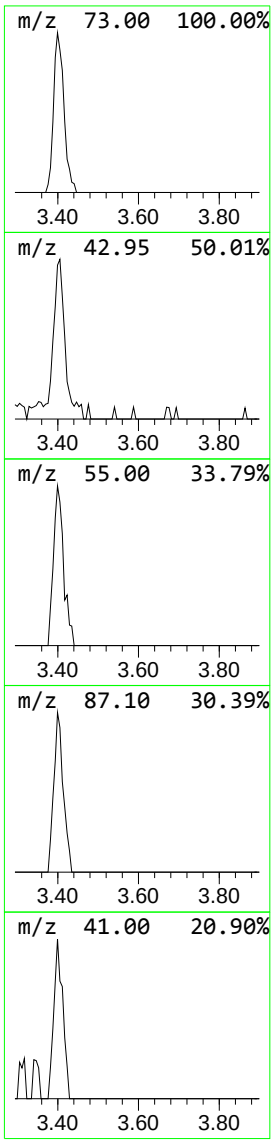
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.400	7.67 ng	20194	1,4-Dichlorobenzene-d4	8.364

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
3	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
4	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	7
5	Isobutylamine	73	C4H11N	000078-81-9	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
Data File : BG056018.D
Acq On : 19 Dec 2022 18:08
Operator : CG/JU
Sample : N6089-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-24

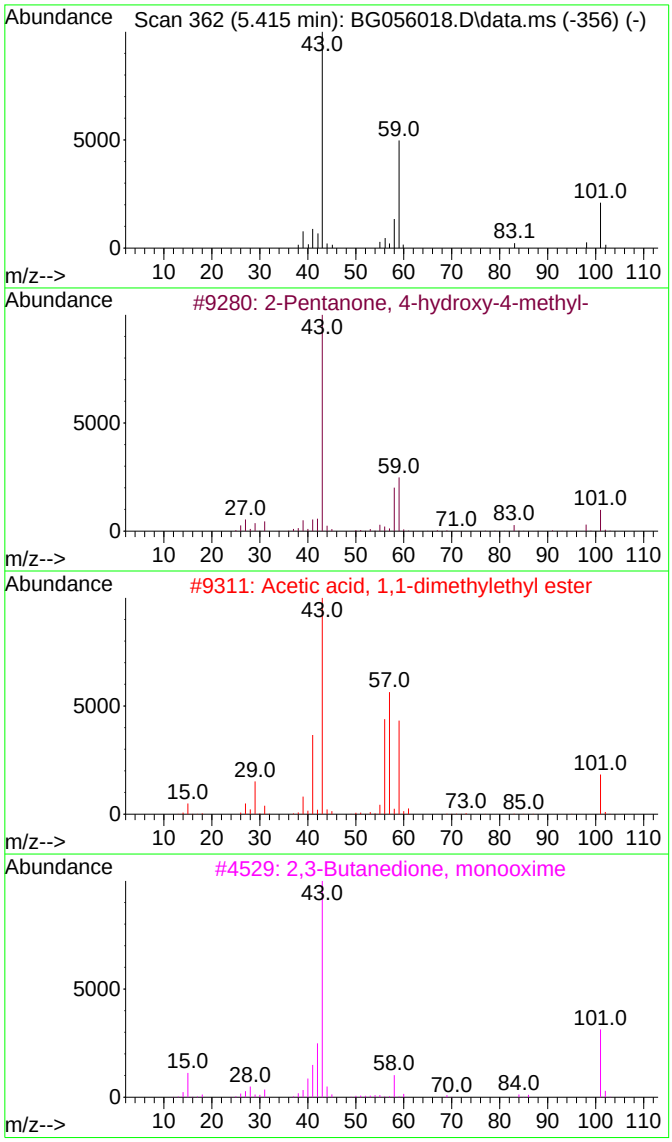
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

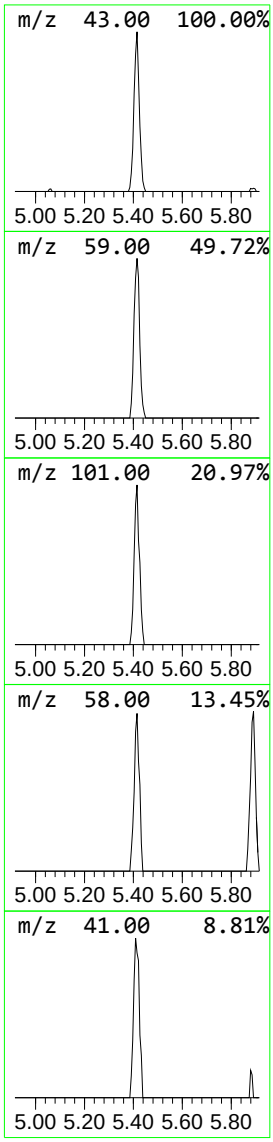
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.415	15.32 ng	40354	1,4-Dichlorobenzene-d4	8.364

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
Data File : BG056018.D
Acq On : 19 Dec 2022 18:08
Operator : CG/JU
Sample : N6089-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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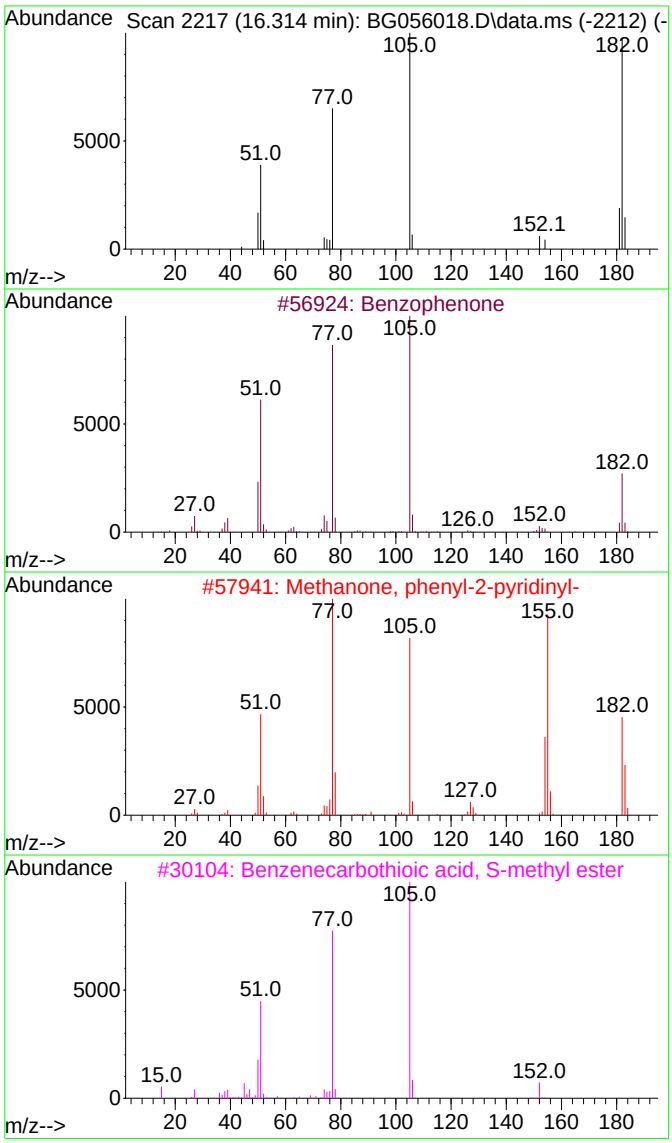
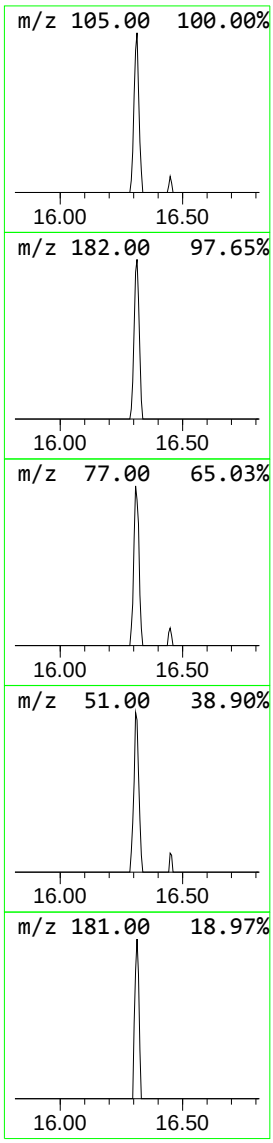
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.314	3.72 ng	21351	Acenaphthene-d10	14.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	91
2	Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	47
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	43
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	38
5	5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
Data File : BG056018.D
Acq On : 19 Dec 2022 18:08
Operator : CG/JU
Sample : N6089-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

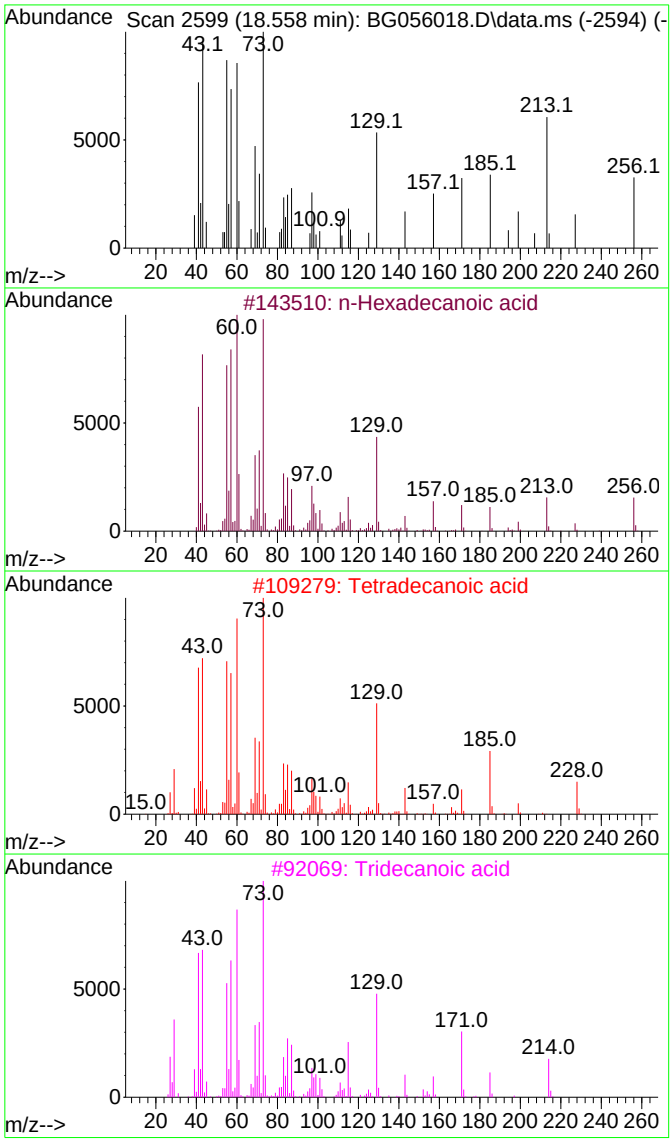
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

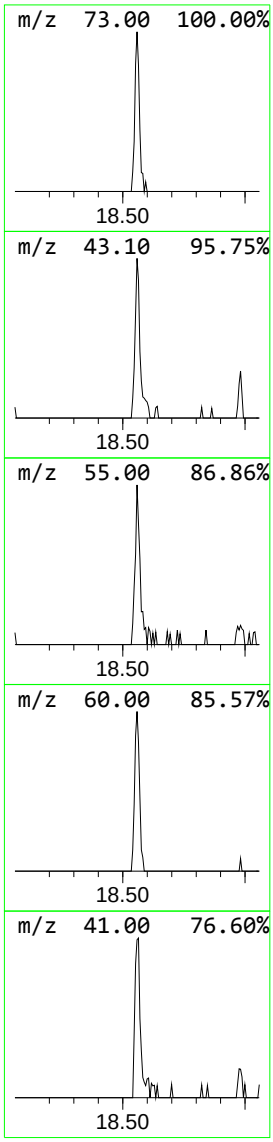
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.558	5.37 ng	44270	Phenanthrene-d10	17.712

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Tridecanoic acid	214	C13H26O2	000638-53-9	52
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
Data File : BG056018.D
Acq On : 19 Dec 2022 18:08
Operator : CG/JU
Sample : N6089-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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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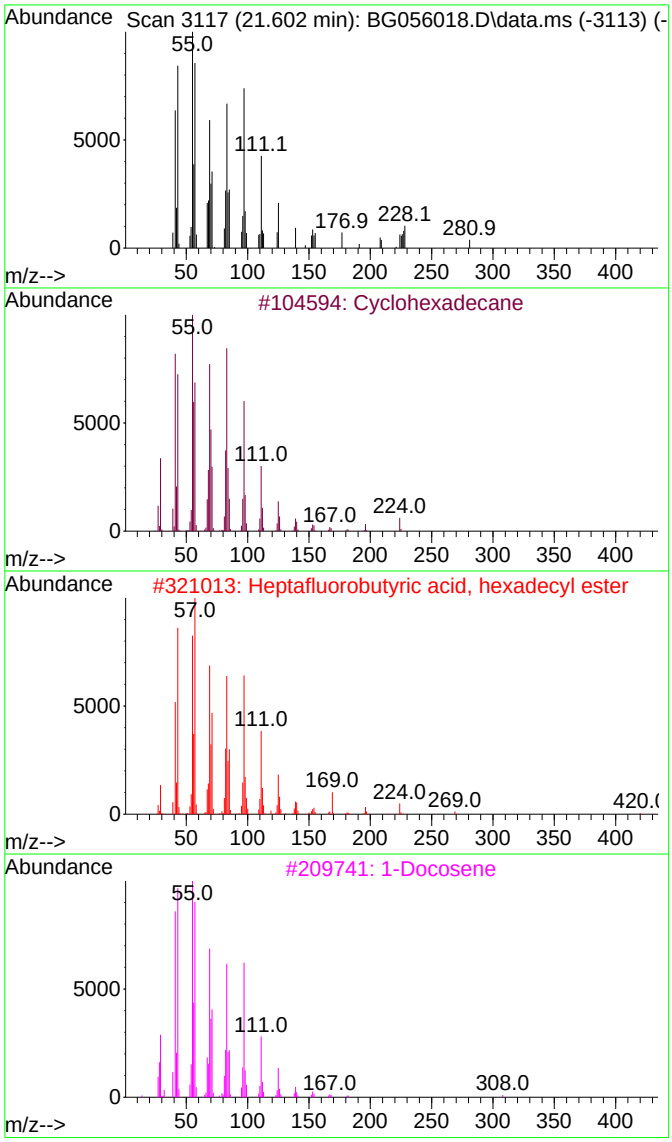
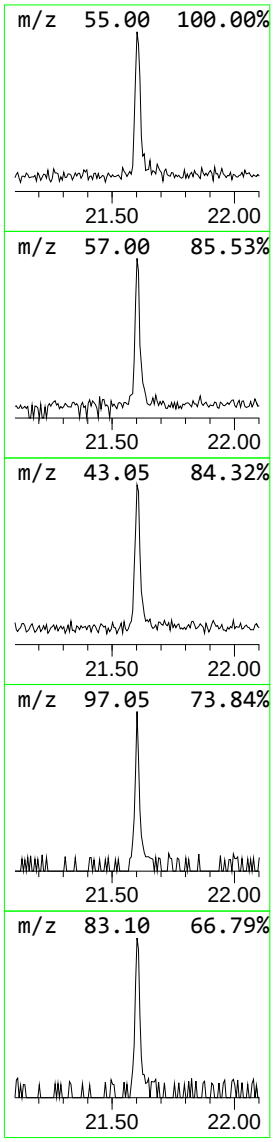
Peak Number 5 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.602	3.59 ng	38997	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	91
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	1-Docosene	308	C22H44	001599-67-3	90
4	1-Tetracosene	336	C24H48	010192-32-2	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





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Sample : N6089-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

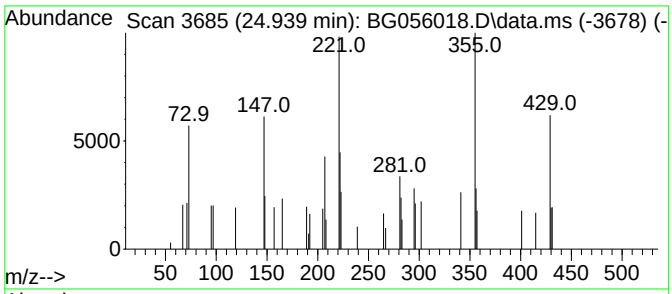
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

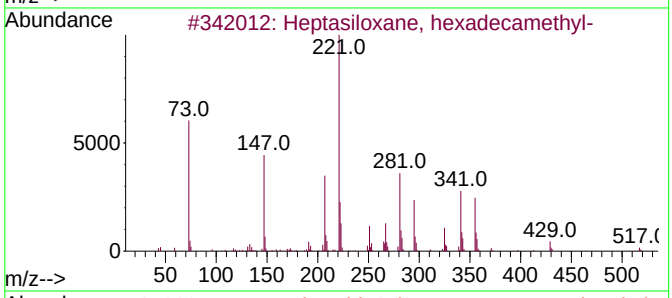
****

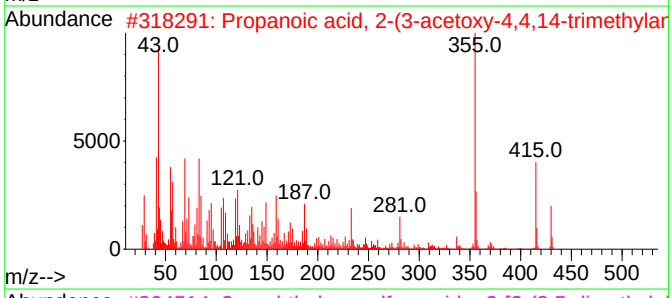
Peak Number 6 unknown24.939 Concentration Rank 7

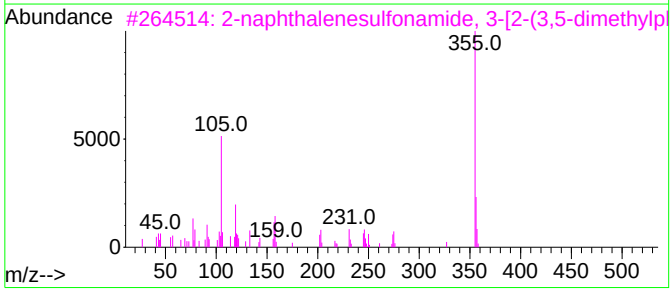
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.939	2.18 ng	23798	Perylene-d12	25.509

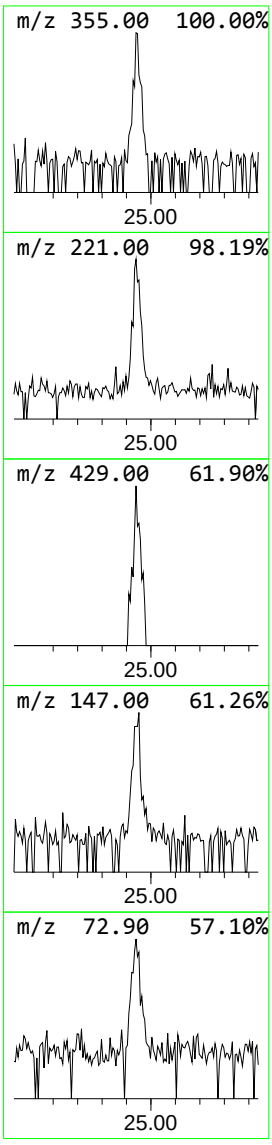
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	32
2	Propanoic acid, 2-(3-acetoxy-4,4...	430	C27H42O4	1000194-01-2	25
3	2-naphthalenesulfonamide, 3-[2-(...	355	C18H17N3O3S	1000398-41-4	14
4	3,4-Dihydroxyphenylglycol, 4TMS ...	458	C20H42O4Si4	056114-62-6	14
5	6H-Dibenzo[a,g]quinolizine, 5,8,...	355	C21H25NO4	002934-97-6	14











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Operator : CG/JU
Sample : N6089-01
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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

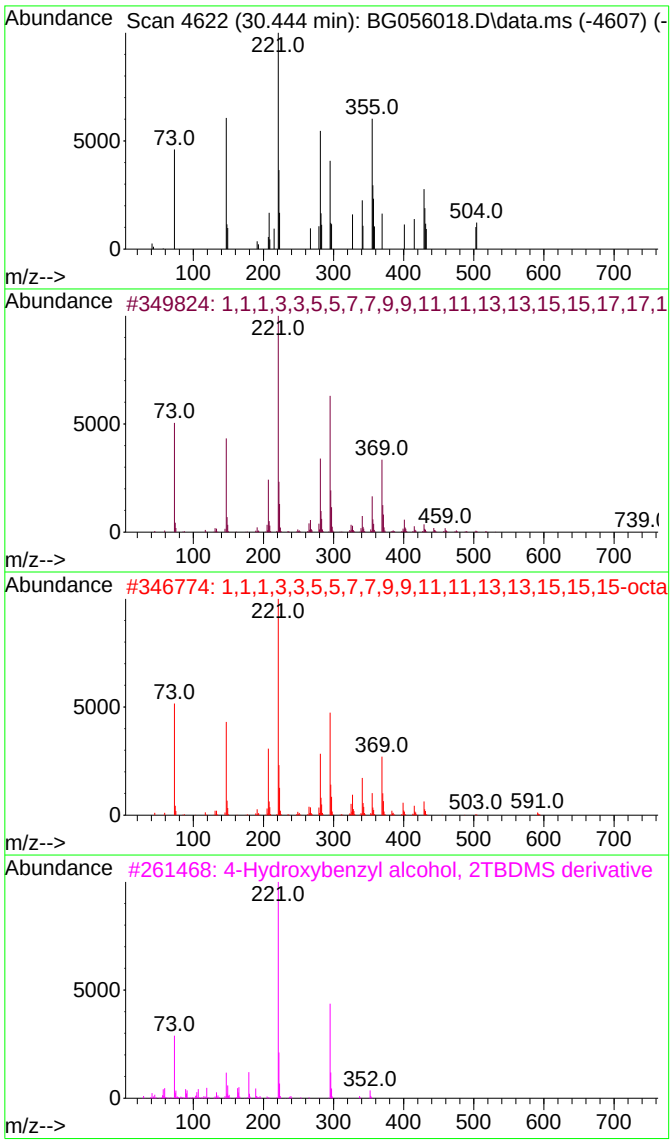
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

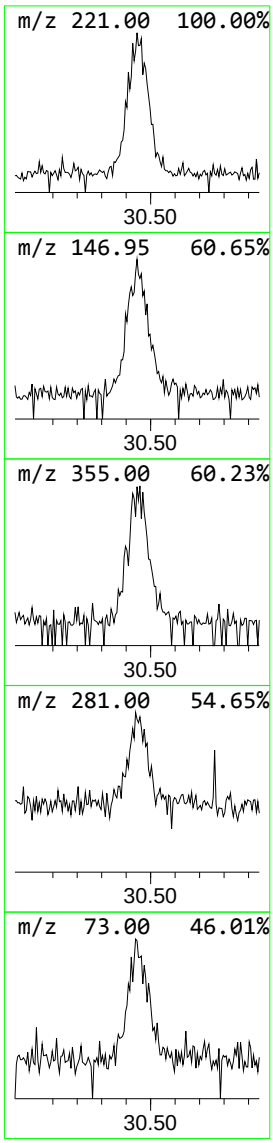
****

Peak Number 7 unknown30.444 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.444	4.46 ng	48795	Perylene-d12	25.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	754	C22H66O9Si10	000556-70-7	38
2	1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	38
3	4-Hydroxybenzyl alcohol, 2TBDMS ...	352	C19H36O2Si2	1000364-43-9	17
4	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	16
5	1,3-Benzodioxole, 5-[3-acetamino...	221	C12H15NO3	1000124-33-0	10





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
Butane, 2-metho...	3.400	7.7	ng	20194	1	8.364	52691	20.0
2-Pentanone, 4-...	5.415	15.3	ng	40354	1	8.364	52691	20.0
Benzophenone	16.314	3.7	ng	21351	3	14.974	114823	20.0
n-Hexadecanoic ...	18.558	5.4	ng	44270	4	17.712	164747	20.0
Cyclohexadecane	21.602	3.6	ng	38997	5	22.019	217510	20.0
unknown24.939	24.939	2.2	ng	23798	6	25.509	218663	20.0
unknown30.444	30.444	4.5	ng	48795	6	25.509	218663	20.0