LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056340.D
Acq On : 18 Jan 2023 22:54
Operator : CG/JU
Sample : 01180-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MH-7

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: BG056340.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.317	3	5	19	rVB	120796	155640	5.83%	1.299%
2	5.344	344	350	357	rBV	112497	171322	6.42%	1.430%
3	5.826	424	432	441	rBV	466137	745997	27.95%	6.228%
4	7.442	698	707	719	rBV	462574	814896	30.53%	6.803%
5	8.306	846	854	862	rBB	127732	215808	8.09%	1.802%
6	9.481	1046	1054	1062	rBB	264534	490188	18.37%	4.092%
7	11.138	1328	1336	1346	rBB	175023	309442	11.59%	2.583%
8	13.546	1738	1746	1753	rBV	1048499	1632849	61.18%	13.631%
9	14.915	1972	1979	1987	rVB	343094	528831	19.81%	4.415%
10	16.255	2199	2207	2215	rVB	194907	269376	10.09%	2.249%
11	16.396	2224	2231	2240	rBV	843253	1249473	46.81%	10.431%
12	17.653	2438	2445	2455	rBV	483003	717208	26.87%	5.987%
13	18.499	2585	2589	2600	rBV	88296	130444	4.89%	1.089%
14	19.757	2799	2803	2806	rBV4	19167	27158	1.02%	0.227%
15	20.233	2877	2884	2889	rBV	2009907	2668972	100.00%	22.280%
16	21.525	3099	3104	3110	rBV	105966	163845	6.14%	1.368%
17	21.948	3169	3176	3184	rVB2	443159	784060	29.38%	6.545%
18	23.688	3467	3472	3481	rVB2	46844	101381	3.80%	0.846%
19	25.386	3749	3761	3772	rBV2	261538	802075	30.05%	6.696%

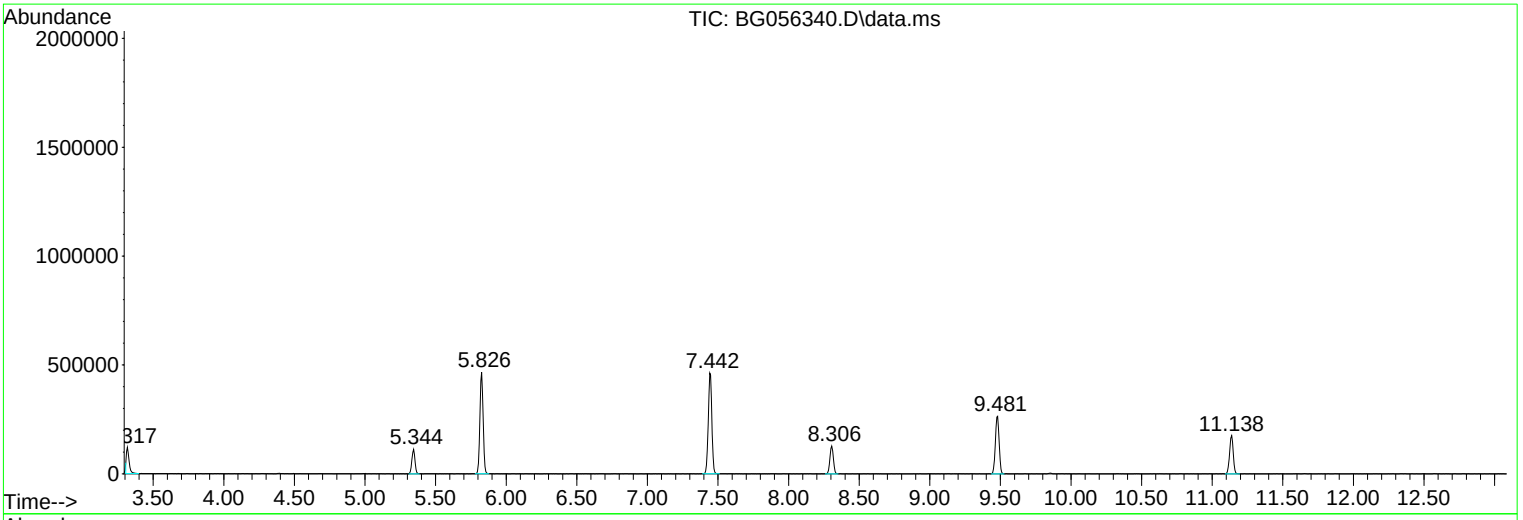
Sum of corrected areas: 11978965

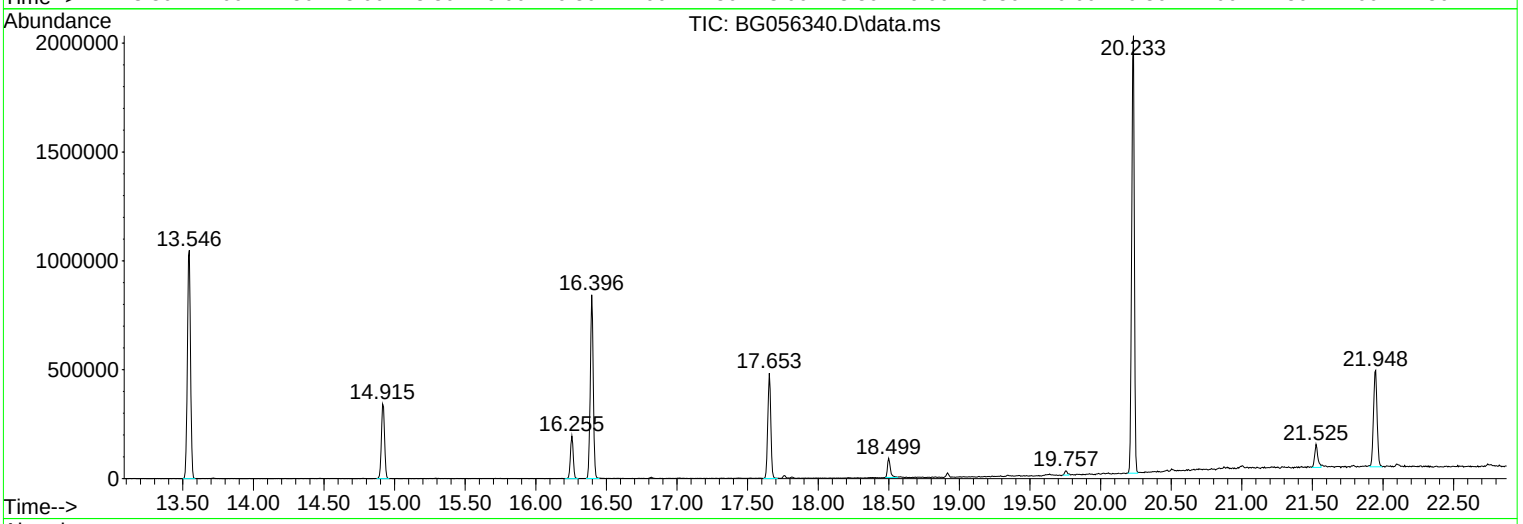
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056340.D
Acq On : 18 Jan 2023 22:54
Operator : CG/JU
Sample : 01180-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

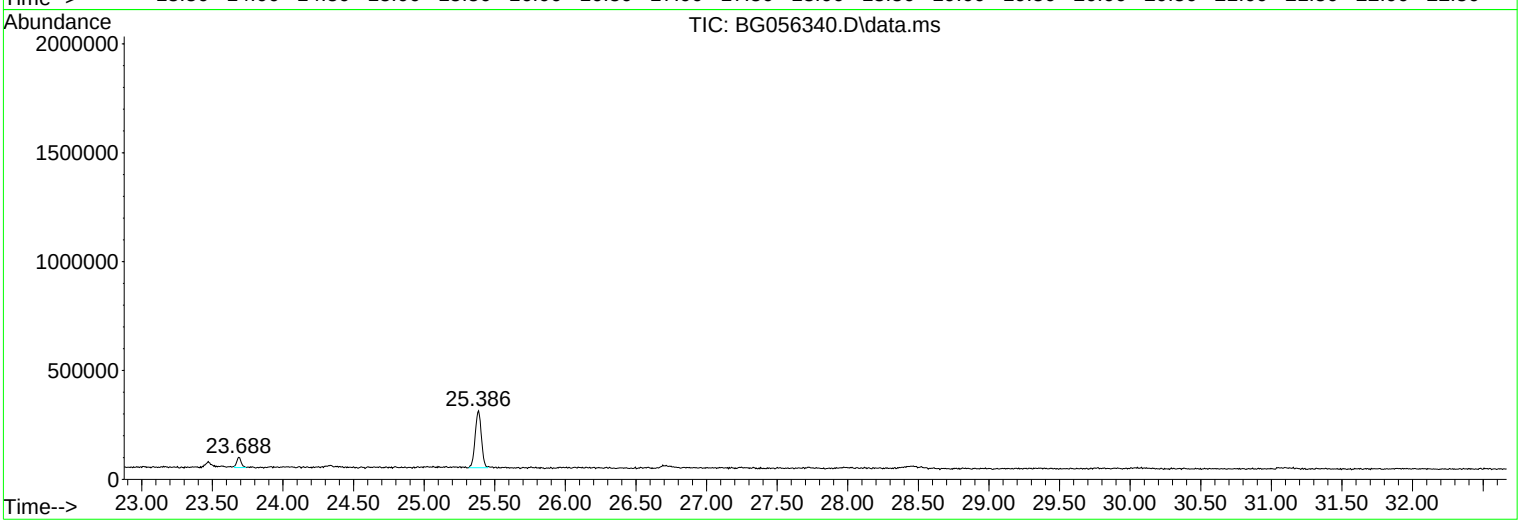
Instrument :
BNA_G
ClientSampleId :
MH-7

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056340.D
Acq On : 18 Jan 2023 22:54
Operator : CG/JU
Sample : 01180-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-7

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

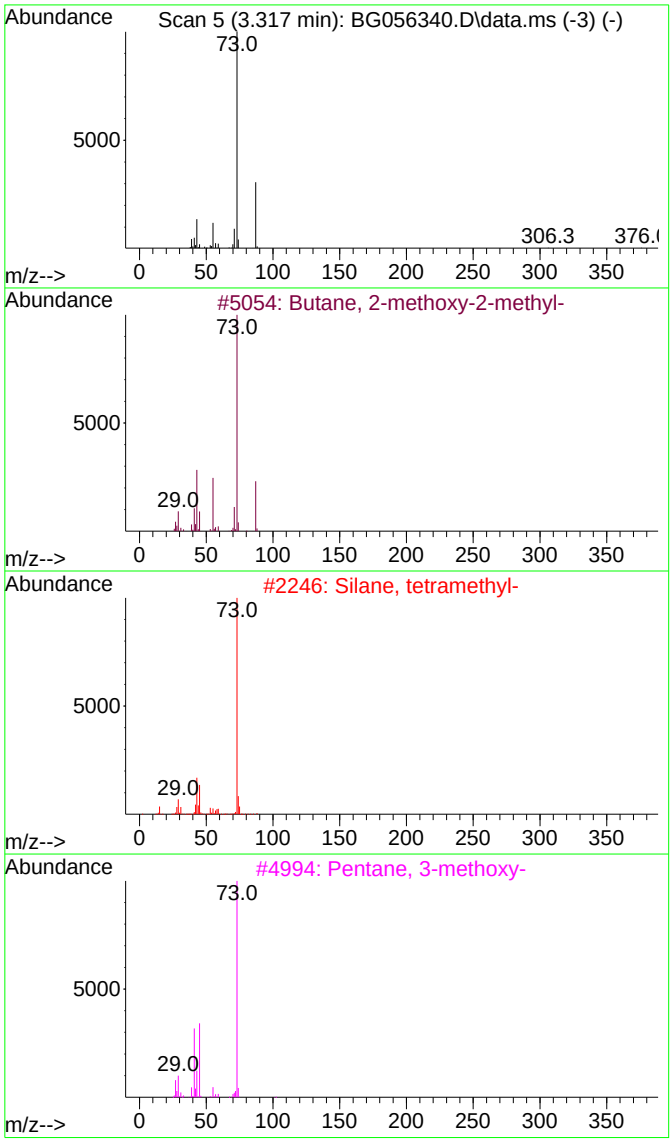
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

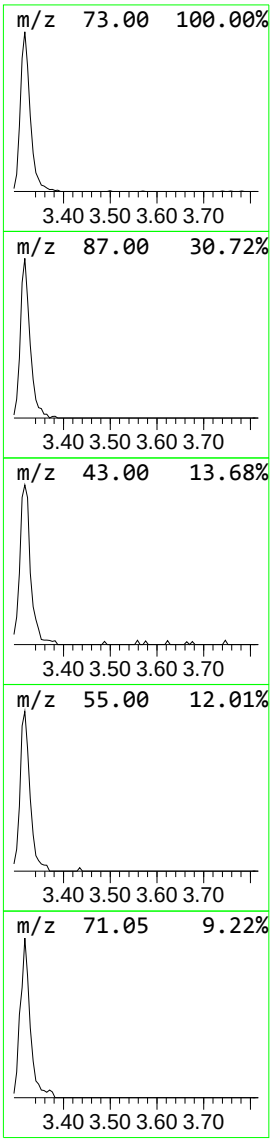
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.317	14.42 ng	155640	1,4-Dichlorobenzene-d4	8.306

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056340.D
Acq On : 18 Jan 2023 22:54
Operator : CG/JU
Sample : 01180-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-7

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

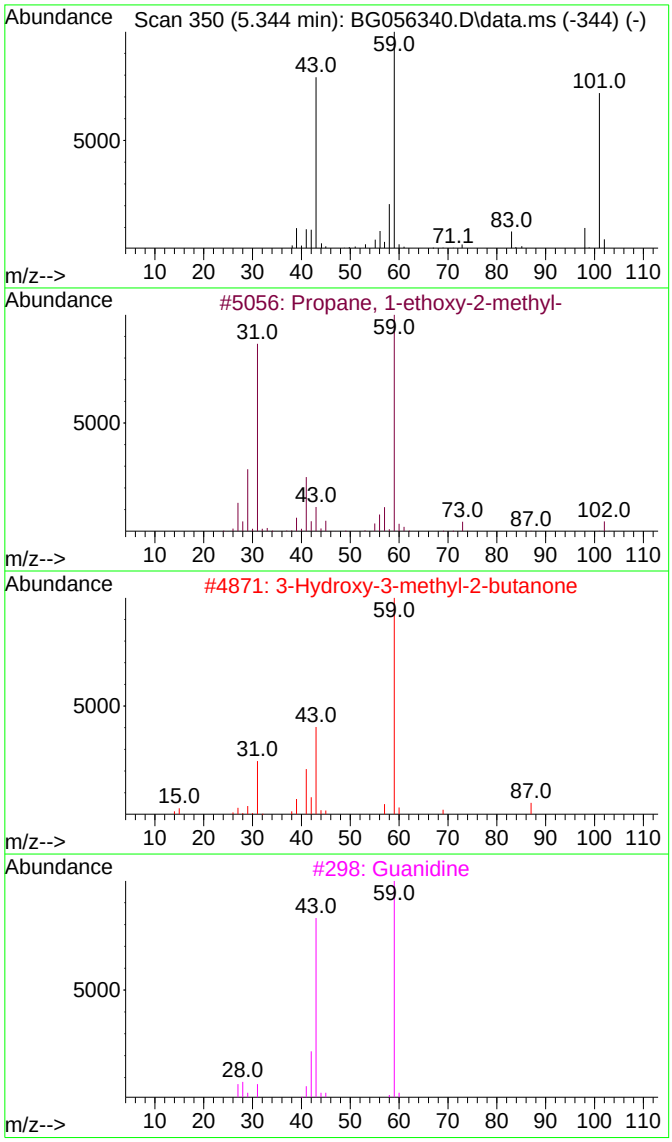
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

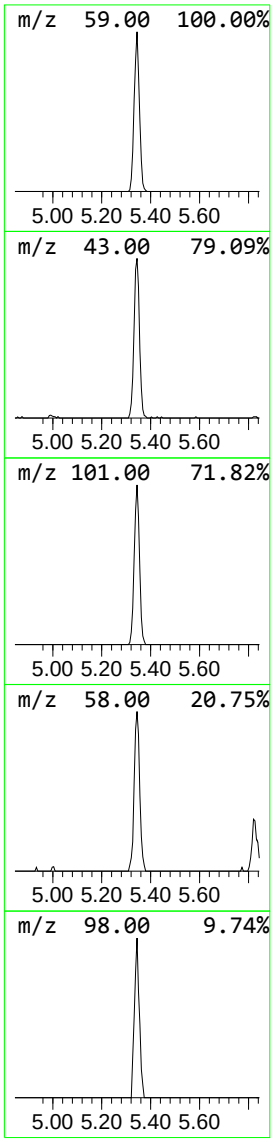
****

Peak Number 2 unknown5.344 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.344	15.88 ng	171322	1,4-Dichlorobenzene-d4	8.306

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3	Guanidine	59	CH5N3	000113-00-8	25
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	23
5	Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056340.D
Acq On : 18 Jan 2023 22:54
Operator : CG/JU
Sample : 01180-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-7

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

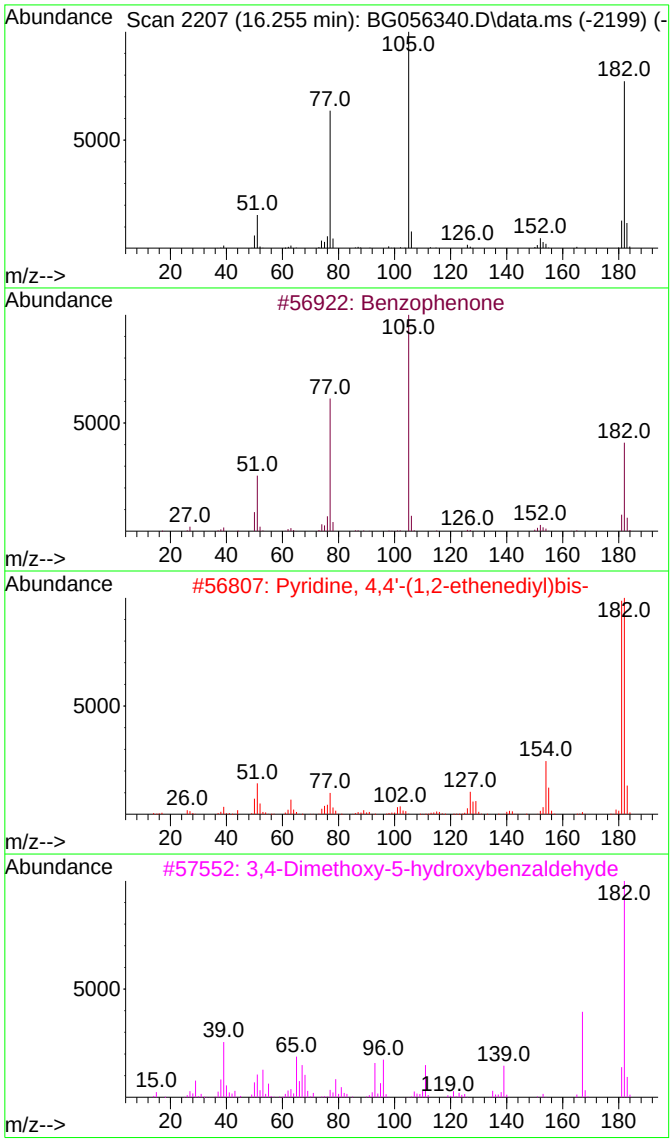
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

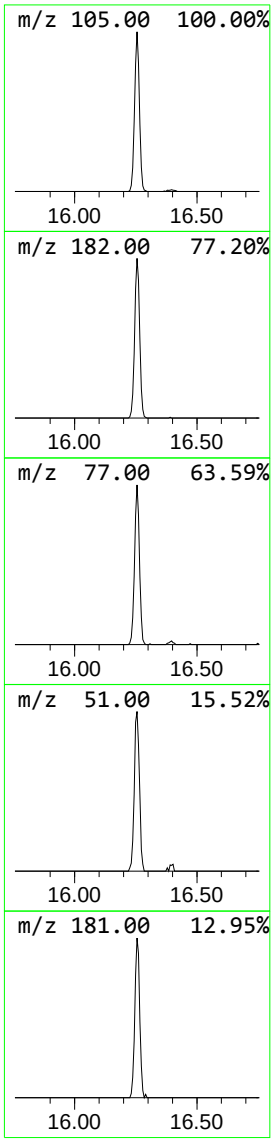
****

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.255	10.19 ng	269376	Acenaphthene-d10	14.915

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Pyridine, 4,4'-(1,2-ethenediyl)bis-	182	C12H10N2	001135-32-6	47
3	3,4-Dimethoxy-5-hydroxybenzaldehyde	182	C9H10O4	029865-90-5	47
4	1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	46
5	2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056340.D
Acq On : 18 Jan 2023 22:54
Operator : CG/JU
Sample : 01180-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-7

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

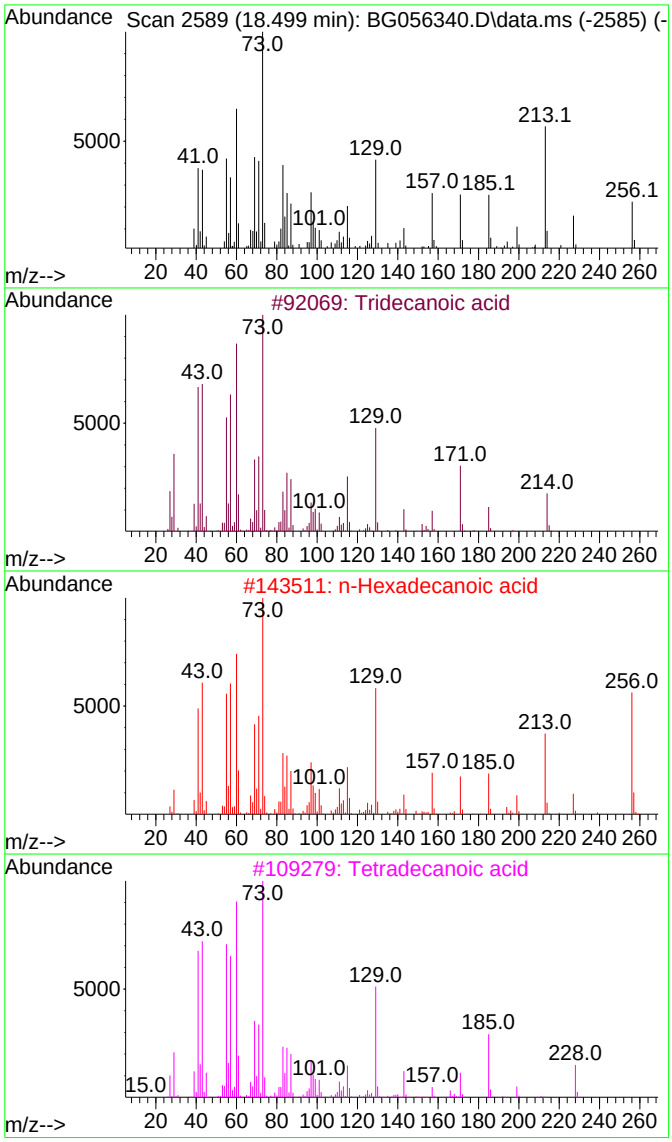
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

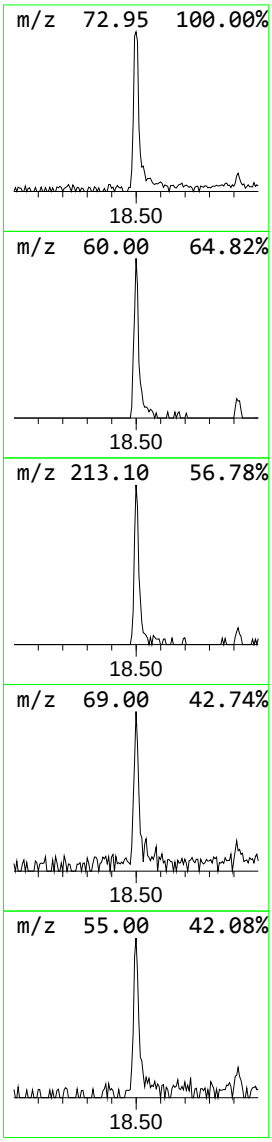
****

Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.500	3.64 ng	130444	Phenanthrene-d10	17.653

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	55
4	Dodecanoic acid	200	C12H24O2	000143-07-7	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056340.D
Acq On : 18 Jan 2023 22:54
Operator : CG/JU
Sample : 01180-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-7

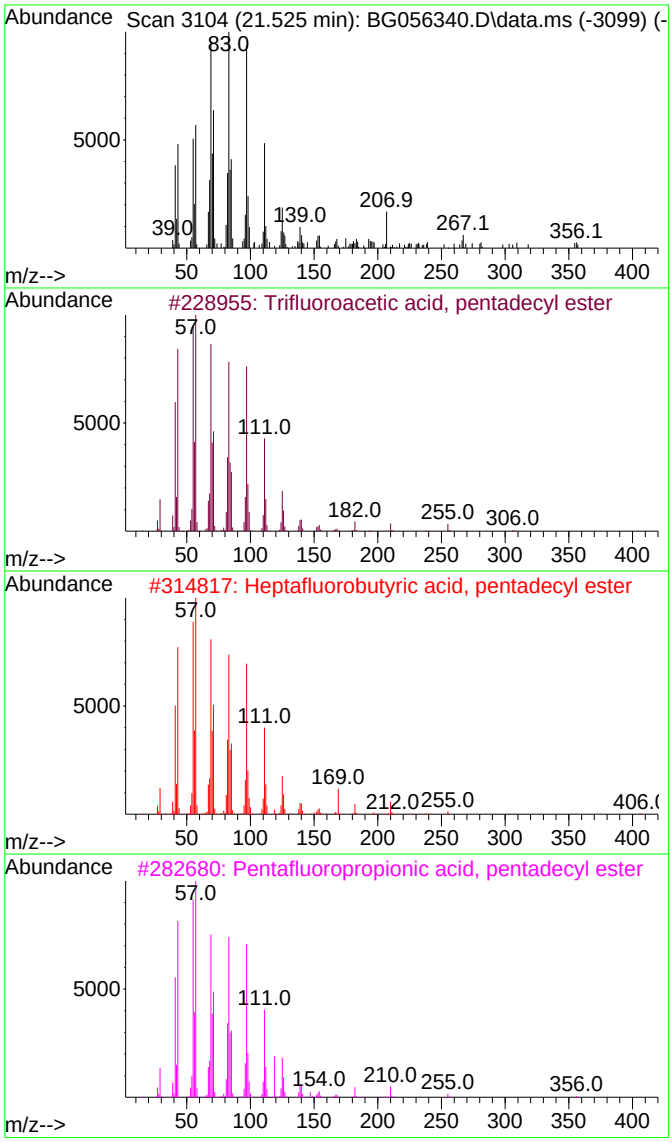
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

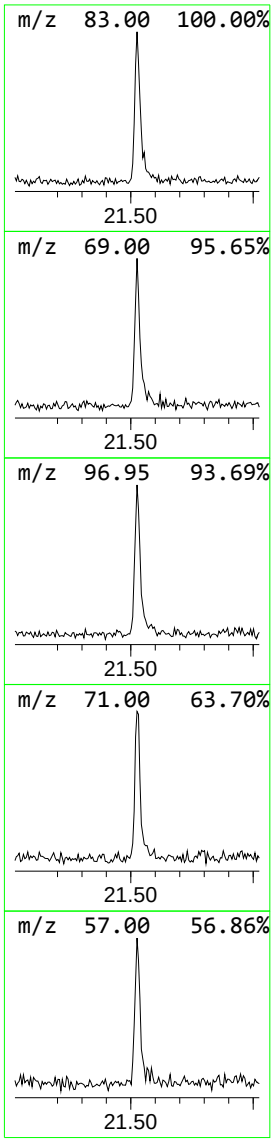
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.525	4.18 ng	163845	Chrysene-d12	21.942

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	1-Hexacosene	364	C26H52	018835-33-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056340.D
Acq On : 18 Jan 2023 22:54
Operator : CG/JU
Sample : 01180-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-7

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

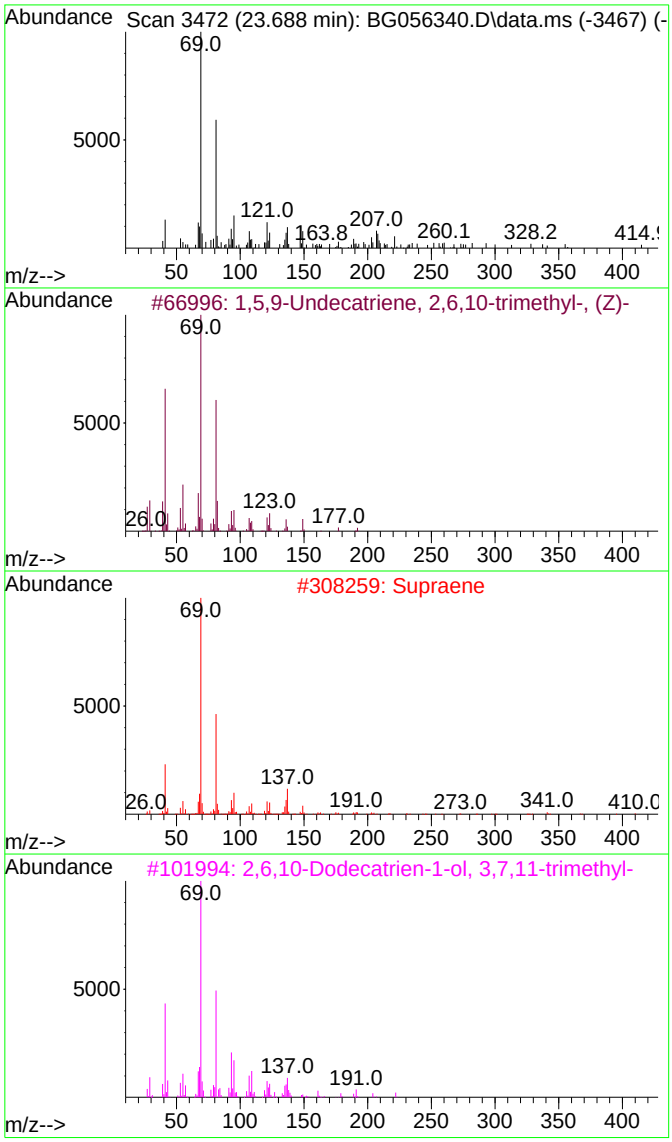
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

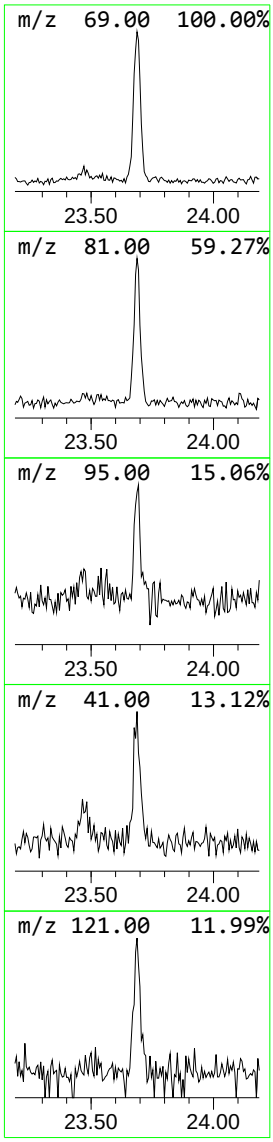
****

Peak Number 6 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.688	2.53 ng	101381	Perylene-d12	25.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
2	Supraene	410	C30H50	007683-64-9	72
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056340.D
Acq On : 18 Jan 2023 22:54
Operator : CG/JU
Sample : 01180-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-7

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.317	14.4	ng	155640	1	8.306	215808	20.0
unknown5.344	5.344	15.9	ng	171322	1	8.306	215808	20.0
Benzophenone	16.255	10.2	ng	269376	3	14.915	528831	20.0
Tridecanoic acid	18.500	3.6	ng	130444	4	17.653	717208	20.0
Trifluoroacetic...	21.525	4.2	ng	163845	5	21.942	784060	20.0
1,5,9-Undecatri...	23.688	2.5	ng	101381	6	25.380	802075	20.0