LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121922\
Data File : BG056014.D
Acq On : 19 Dec 2022 15:23
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

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: BG056014.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	25	rBV	21539	29358	3.51%	0.832%
2	5.409	356	361	368	rBB	14163	21951	2.63%	0.622%
3	5.885	436	442	449	rBB	130097	201553	24.13%	5.710%
4	7.495	709	716	723	rBB	128970	224144	26.83%	6.350%
5	8.370	858	865	871	rBB	32624	53884	6.45%	1.527%
6	9.540	1057	1064	1071	rBB	79812	138935	16.63%	3.936%
7	11.202	1340	1347	1354	rBB	44189	77389	9.26%	2.192%
8	13.606	1749	1756	1762	rBB	276220	424945	50.87%	12.039%
9	14.975	1983	1989	1995	rBB	88514	132513	15.86%	3.754%
10	16.308	2210	2216	2223	rBB	31313	45987	5.51%	1.303%
11	16.449	2234	2240	2247	rBV	359908	523421	62.66%	14.829%
12	17.712	2448	2455	2460	rBV	123659	185664	22.23%	5.260%
13	18.559	2593	2599	2607	rBV	40385	51874	6.21%	1.470%
14	18.982	2667	2671	2674	rBV	14578	15380	1.84%	0.436%
15	19.810	2807	2812	2818	rBV7	13394	19696	2.36%	0.558%
16	20.098	2855	2861	2868	rVB	6117	10459	1.25%	0.296%
17	20.286	2887	2893	2898	rBV	650215	835353	100.00%	23.666%
18	21.602	3113	3117	3122	rVB2	30175	41104	4.92%	1.164%
19	22.019	3181	3188	3196	rVB	133106	232759	27.86%	6.594%
20	25.515	3772	3783	3793	rBV2	83062	263425	31.53%	7.463%

Sum of corrected areas: 3529794

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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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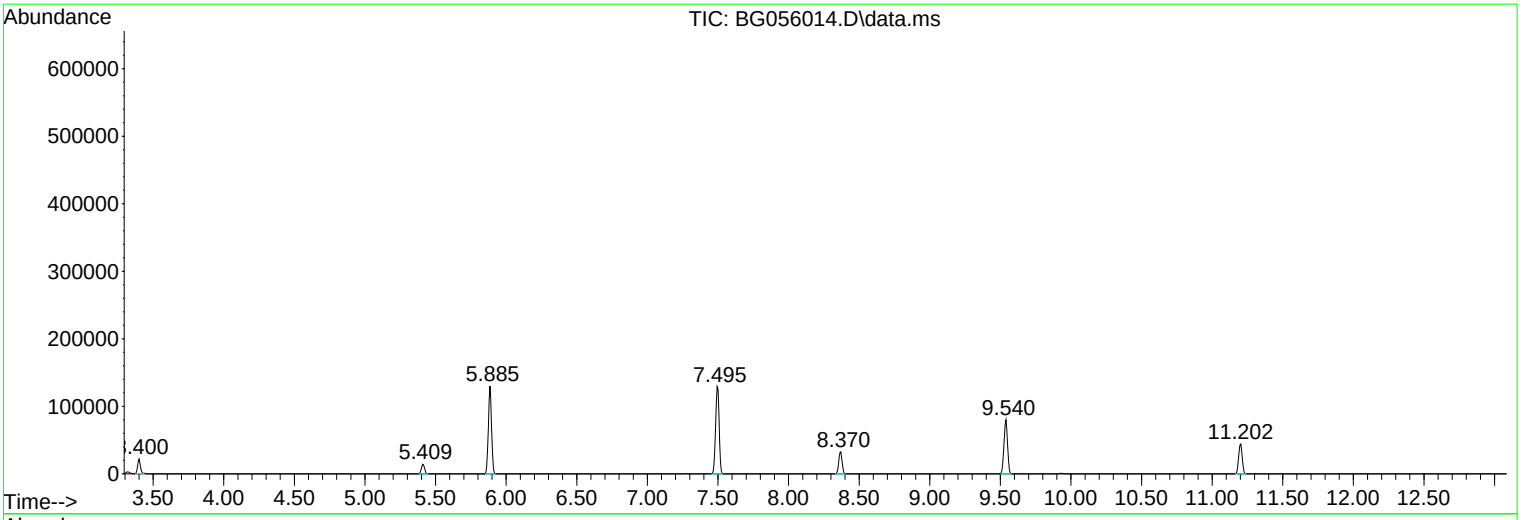
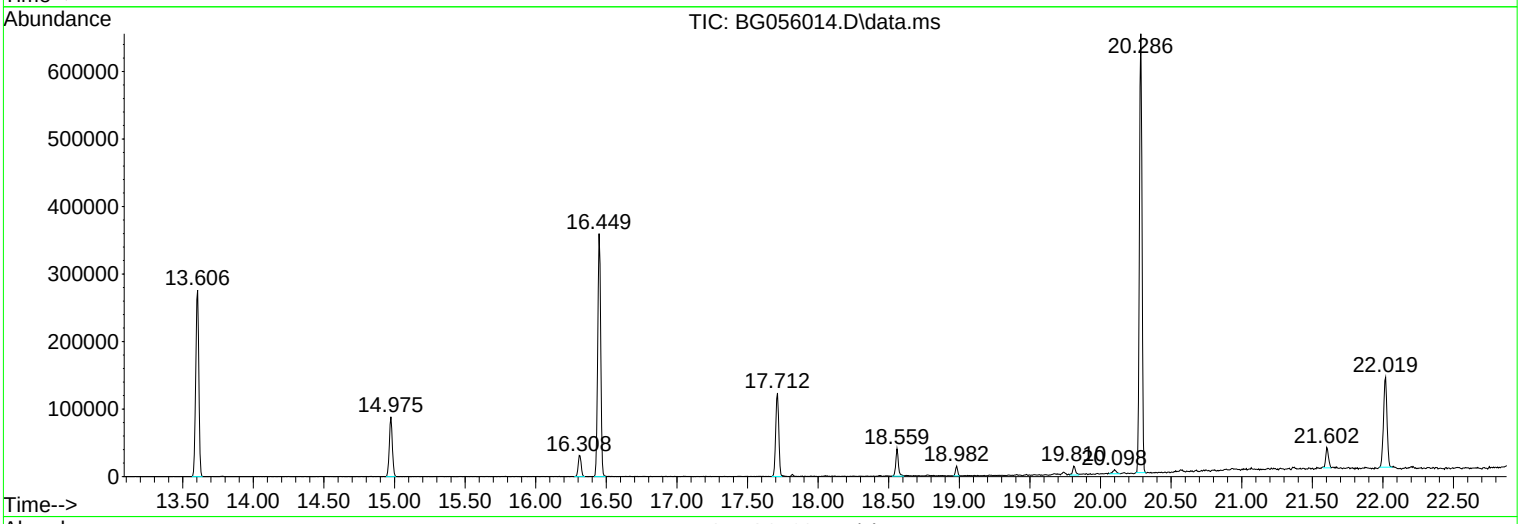
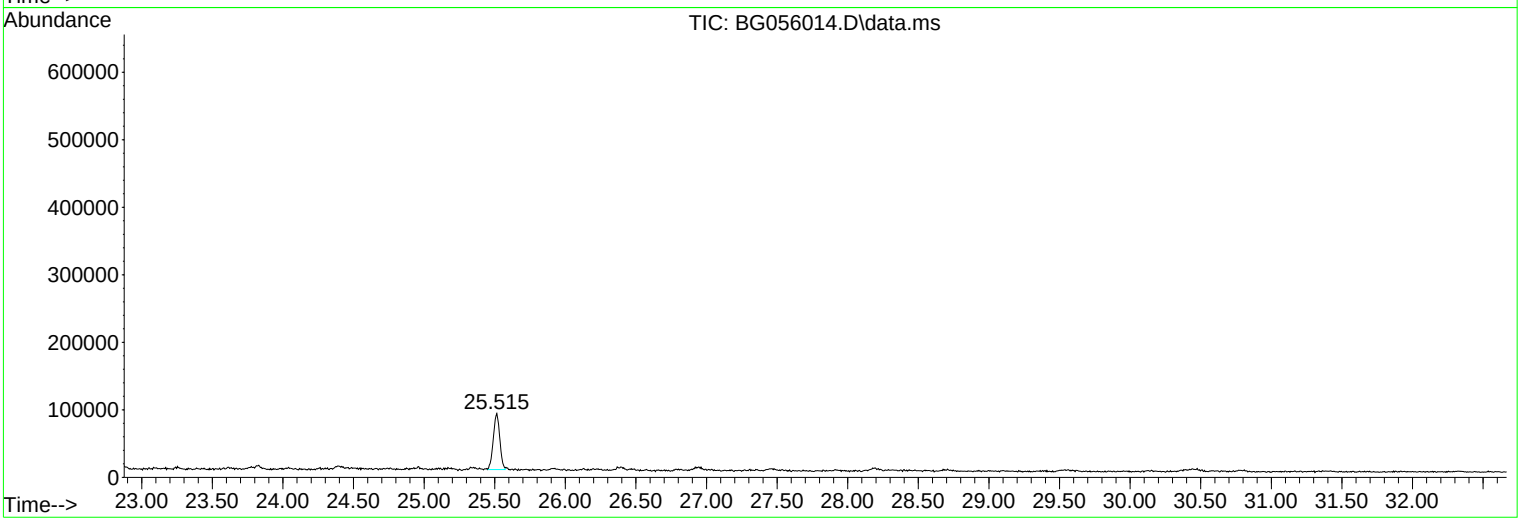
ClientSampleId :
TP-Q

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

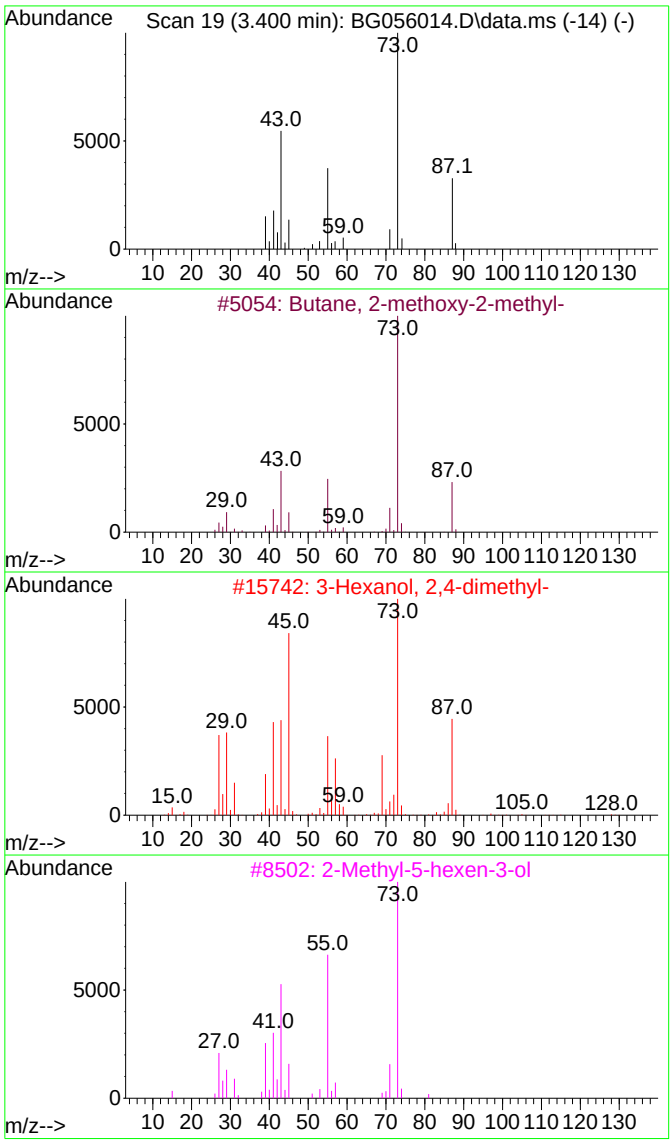
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

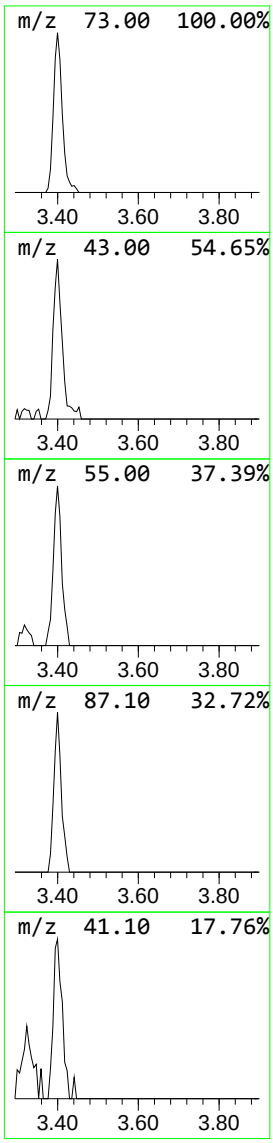
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.400	10.90 ng	29358	1,4-Dichlorobenzene-d4	8.370

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	36
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	(R)-3-Pyrrolidinol	87	C4H9NO	002799-21-5	9





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Operator : CG/JU
Sample : N6024-01
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Instrument :
BNA_G
ClientSampleId :
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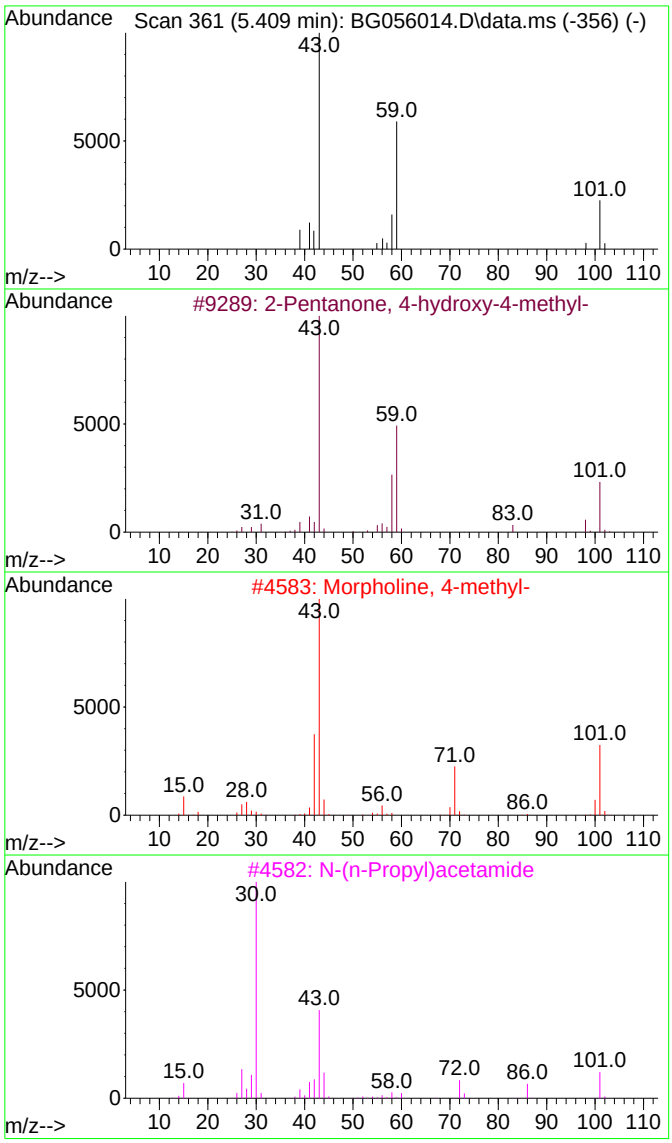
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

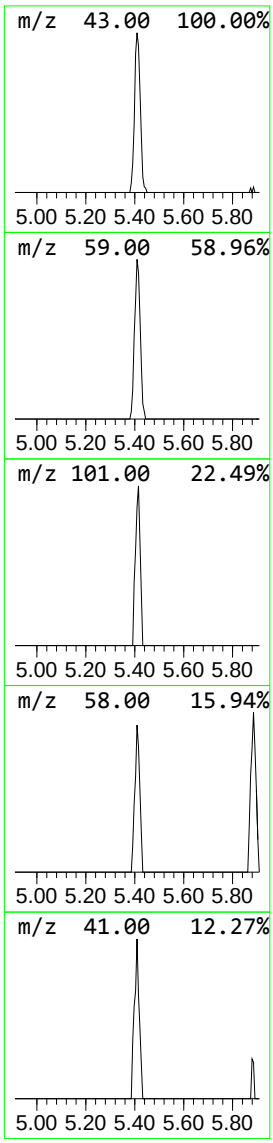
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.409	8.15 ng	21951	1,4-Dichlorobenzene-d4	8.370

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	Butane	58	C4H10	000106-97-8	9





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Data File : BG056014.D
Acq On : 19 Dec 2022 15:23
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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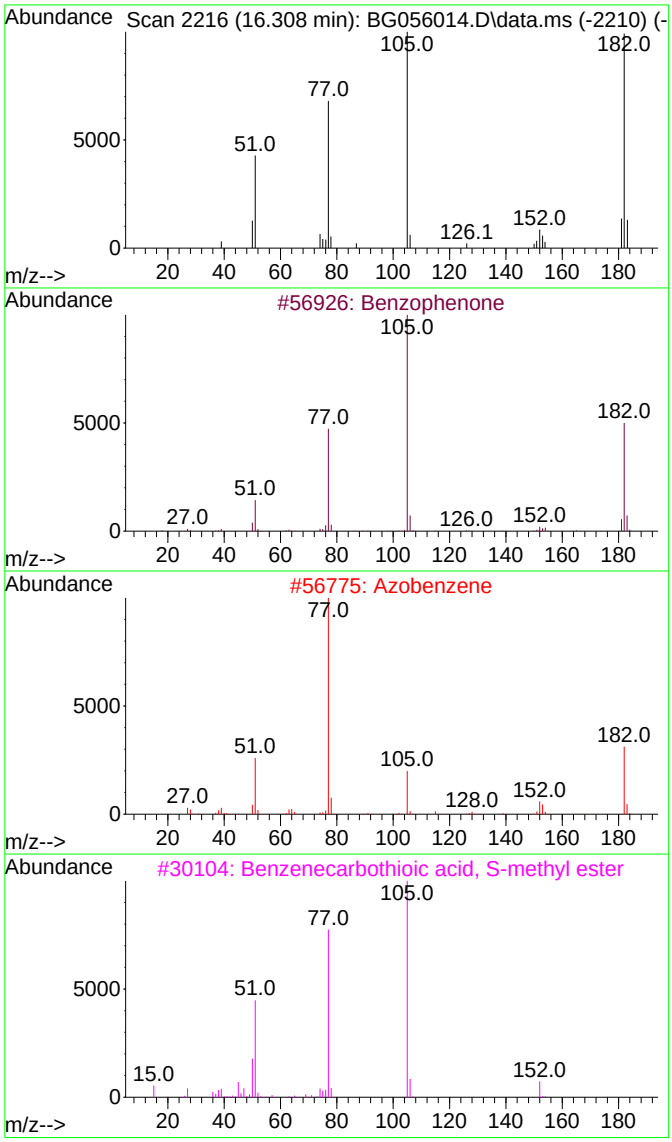
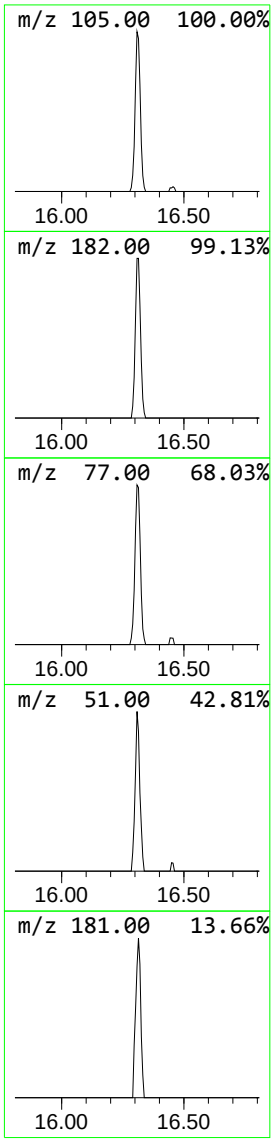
Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.308	6.94 ng	45987	Acenaphthene-d10	14.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	91
2	Azobenzene	182	C12H10N2	000103-33-3	72
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	43
4	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	38
5	Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	38





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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
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TIC Library : C:\Database\NIST20.L
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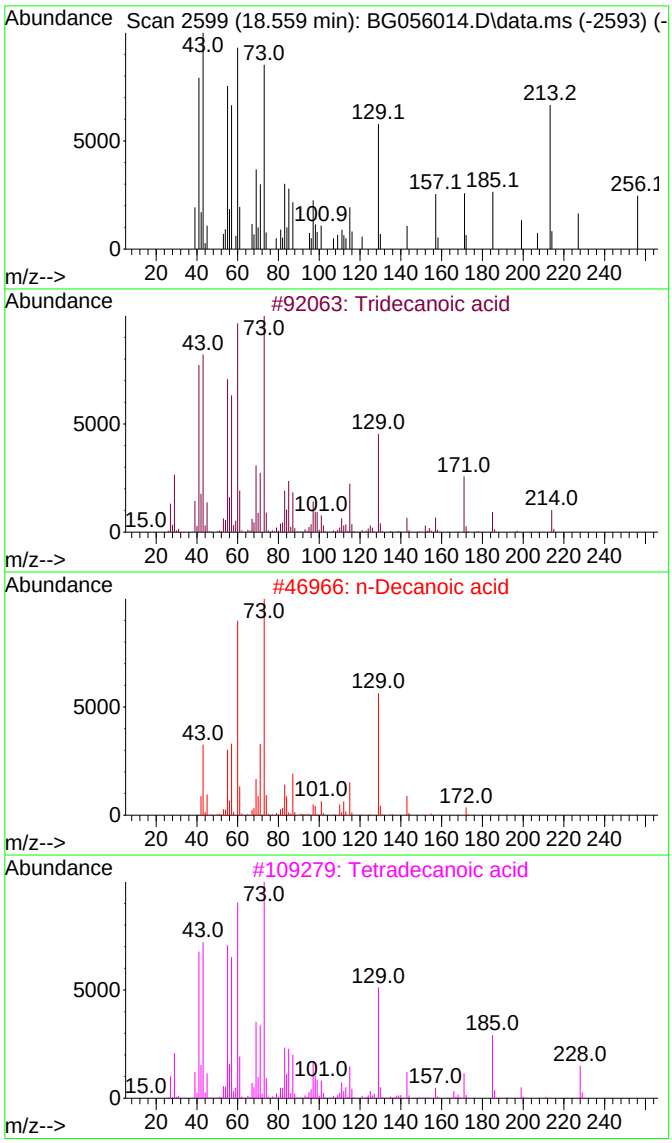
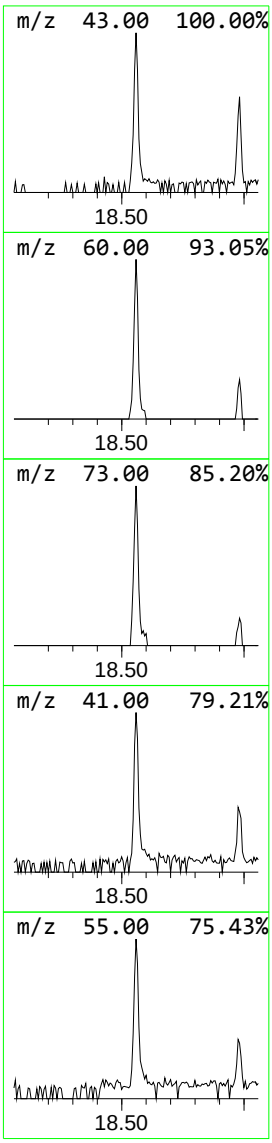
Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.559	5.59 ng	51874	Phenanthrene-d10	17.712

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Decanoic acid	172	C10H20O2	000334-48-5	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	49





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Data File : BG056014.D
Acq On : 19 Dec 2022 15:23
Operator : CG/JU
Sample : N6024-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

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

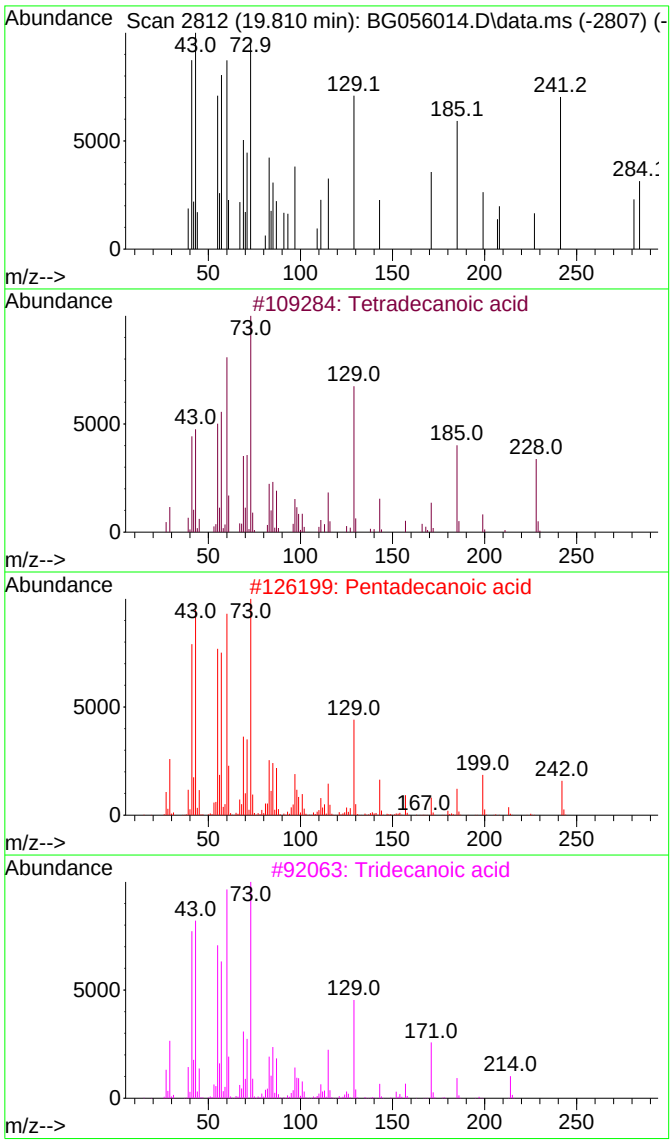
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

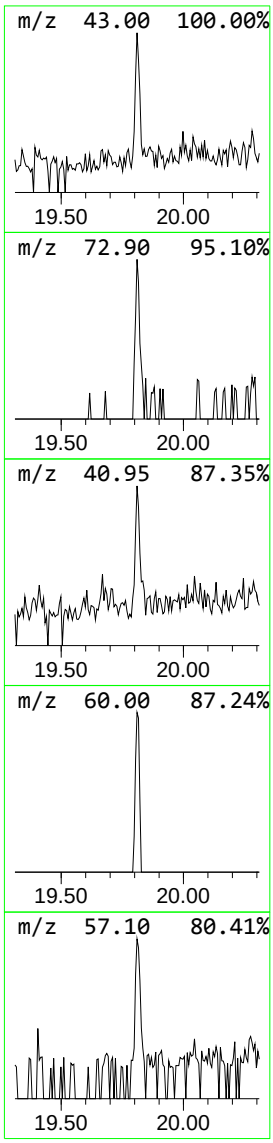
****

Peak Number 5 unknown19.810 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.810	2.12 ng	19696	Phenanthrene-d10	17.712

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
3	Tridecanoic acid	214	C13H26O2	000638-53-9	35
4	Octadecanoic acid	284	C18H36O2	000057-11-4	35
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	25





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-Q

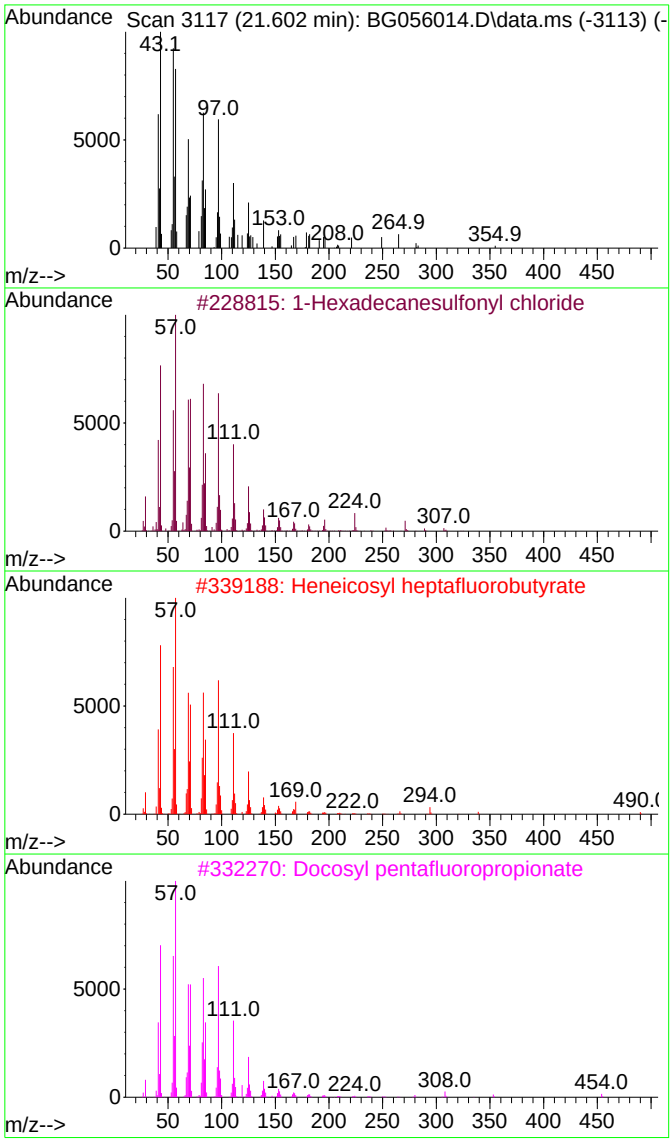
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

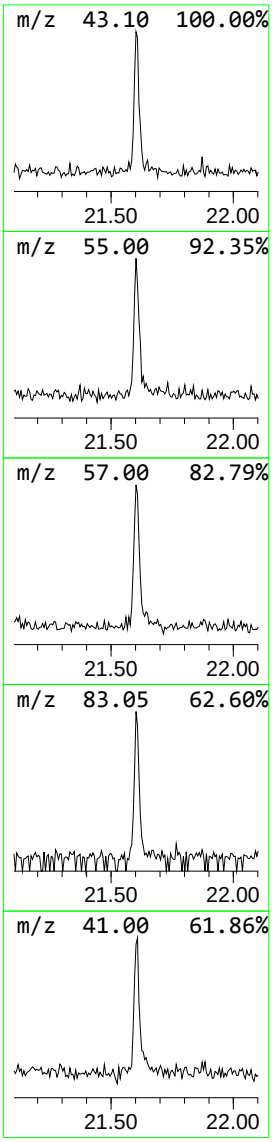
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexadecanesulfonyl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.602	3.53 ng	41104	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
2	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
4	1-Dotriacontanol, acetate	509	C34H68O2	023811-94-1	87
5	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	87





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	10.9	ng	29358	1	8.370	53884	20.0
2-Pentanone, 4-...	5.409	8.2	ng	21951	1	8.370	53884	20.0
Benzophenone	16.308	6.9	ng	45987	3	14.975	132513	20.0
Tridecanoic acid	18.559	5.6	ng	51874	4	17.712	185664	20.0
unknown19.810	19.810	2.1	ng	19696	4	17.712	185664	20.0
1-Hexadecanesul...	21.602	3.5	ng	41104	5	22.019	232759	20.0