LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122322\
Data File : BG056078.D
Acq On : 23 Dec 2022 14:26
Operator : CG/JU
Sample : N6157-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221419-COMPOSITE-B

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: BG056078.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.382	11	16	25	rVB	23953	37185	5.64%	1.170%
2	5.397	353	359	368	rVB	47638	73164	11.10%	2.302%
3	5.873	433	440	448	rVB	121725	193797	29.39%	6.097%
4	7.483	707	714	724	rVB	115537	204239	30.97%	6.425%
5	8.352	857	862	869	rVB	28314	48217	7.31%	1.517%
6	9.527	1054	1062	1069	rBV	71264	124340	18.86%	3.912%
7	11.190	1338	1345	1352	rBV	35864	63047	9.56%	1.983%
8	13.593	1747	1754	1760	rVB	202308	300540	45.58%	9.455%
9	14.968	1980	1988	1994	rBV	69608	105271	15.96%	3.312%
10	16.302	2211	2215	2222	rVB	5462	7664	1.16%	0.241%
11	16.443	2232	2239	2246	rBV	326351	493121	74.78%	15.514%
12	17.700	2447	2453	2462	rVB	115407	172481	26.16%	5.426%
13	18.552	2590	2598	2603	rBV3	26243	39767	6.03%	1.251%
14	19.375	2732	2738	2743	rBV2	7346	16371	2.48%	0.515%
15	19.804	2807	2811	2821	rVB5	13886	24529	3.72%	0.772%
16	19.956	2832	2837	2841	rBV4	4906	6815	1.03%	0.214%
17	20.279	2886	2892	2898	rBV	516084	659418	100.00%	20.745%
18	20.791	2973	2979	2984	rBV3	6528	11778	1.79%	0.371%
19	21.214	3046	3051	3058	rBV3	10612	18540	2.81%	0.583%
20	21.607	3113	3118	3130	rBV4	14219	40143	6.09%	1.263%
21	21.848	3153	3159	3166	rVB8	8806	20124	3.05%	0.633%
22	22.013	3180	3187	3195	rVB2	139187	236132	35.81%	7.429%
23	22.583	3278	3284	3289	rVB5	8112	17621	2.67%	0.554%
24	25.503	3770	3781	3792	rVB3	87270	264304	40.08%	8.315%

Sum of corrected areas: 3178608

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Misc :
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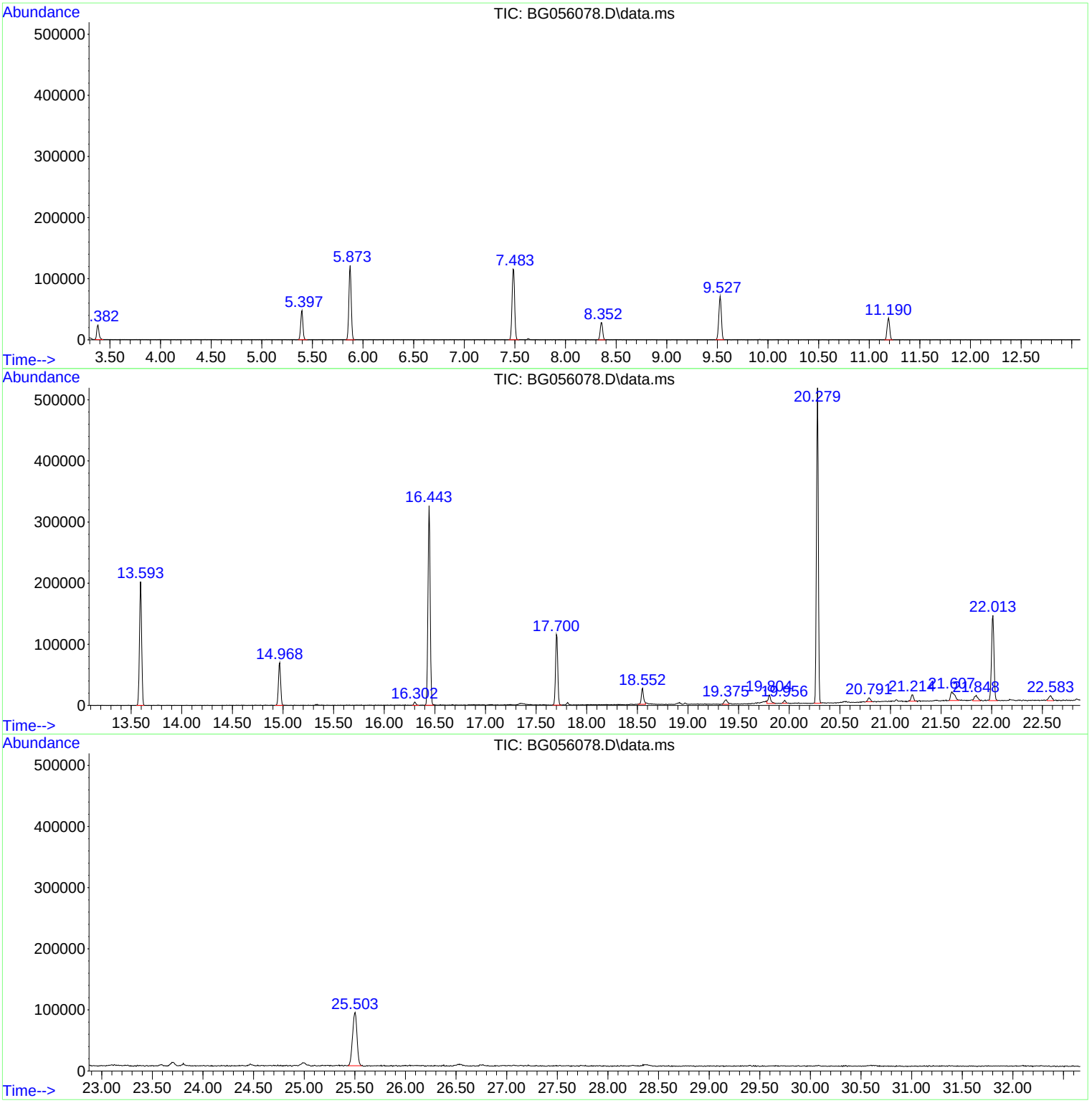
Instrument :
BNA_G
ClientSampleId :
20221419-COMPOSITE-B

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\BG122322\
Data File : BG056078.D
Acq On : 23 Dec 2022 14:26
Operator : CG/JU
Sample : N6157-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221419-COMPOSITE-B

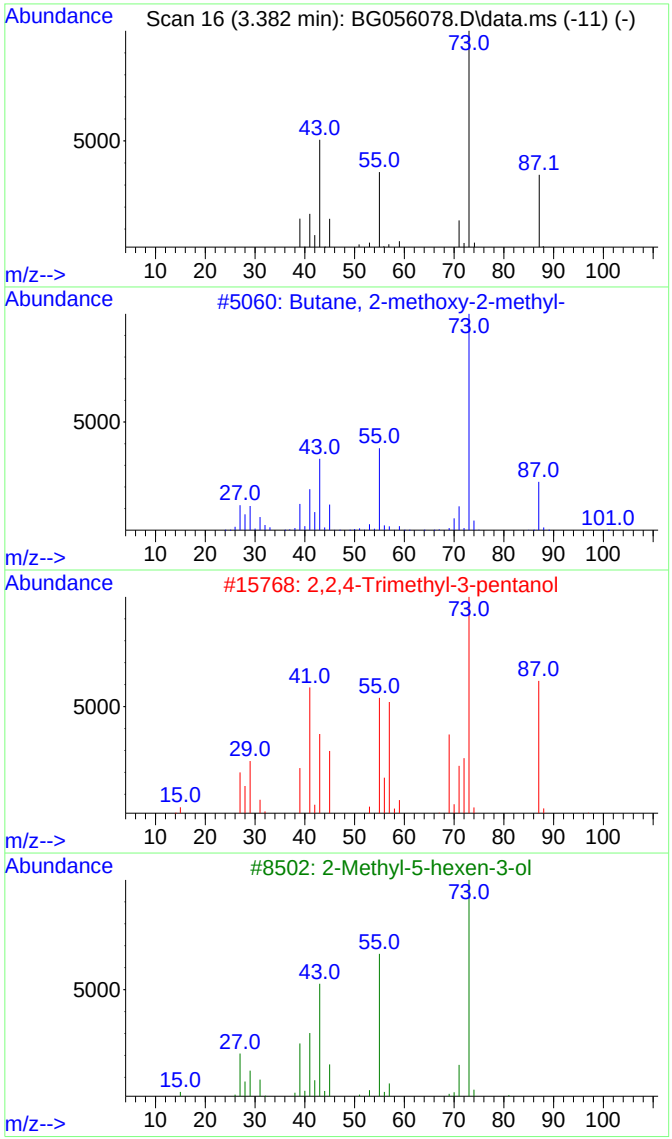
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

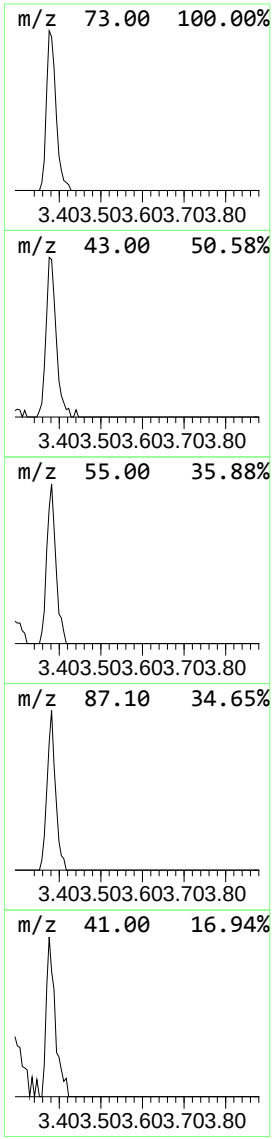
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.382	15.42 ng	37185	1,4-Dichlorobenzene-d4	8.358

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BG056078.D
Acq On : 23 Dec 2022 14:26
Operator : CG/JU
Sample : N6157-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221419-COMPOSITE-B

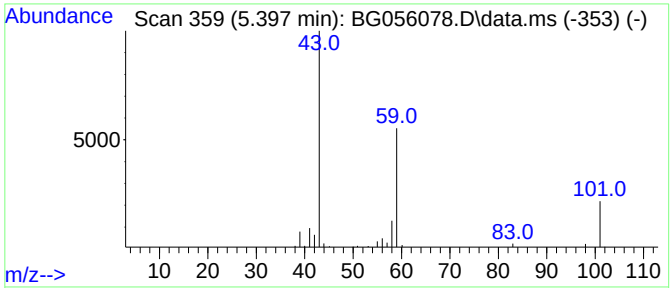
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

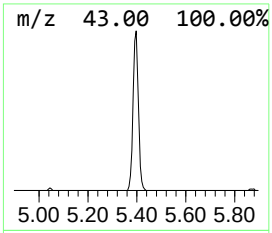
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

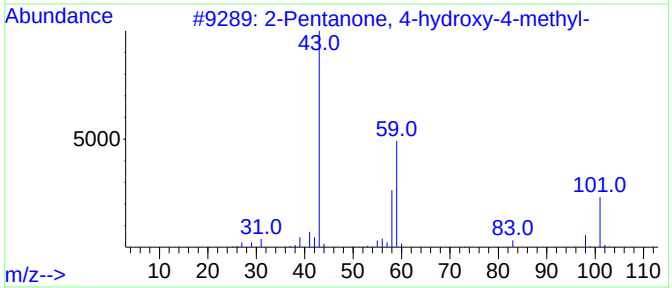
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

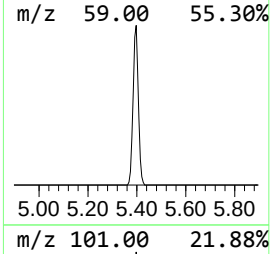
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.397	30.35 ng	73164	1,4-Dichlorobenzene-d4	8.358

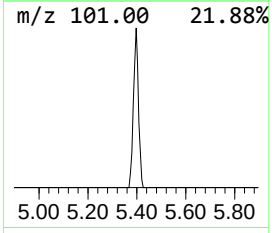
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5	Butane	58	C4H10	000106-97-8	9

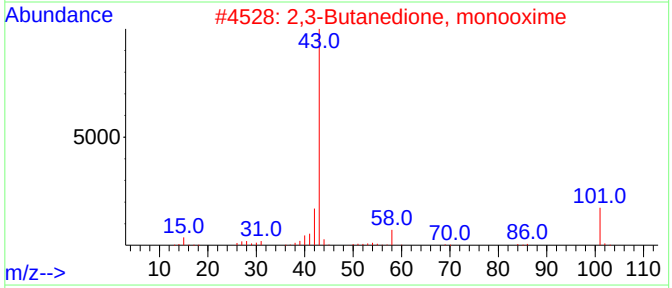


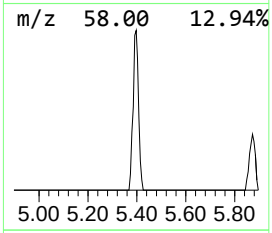


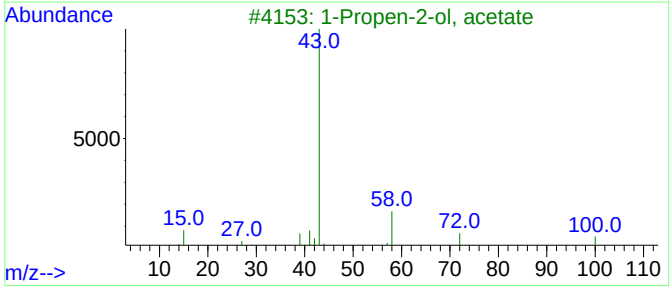


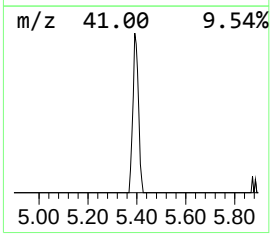












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Instrument :
BNA_G
ClientSampleId :
20221419-COMPOSITE-B

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

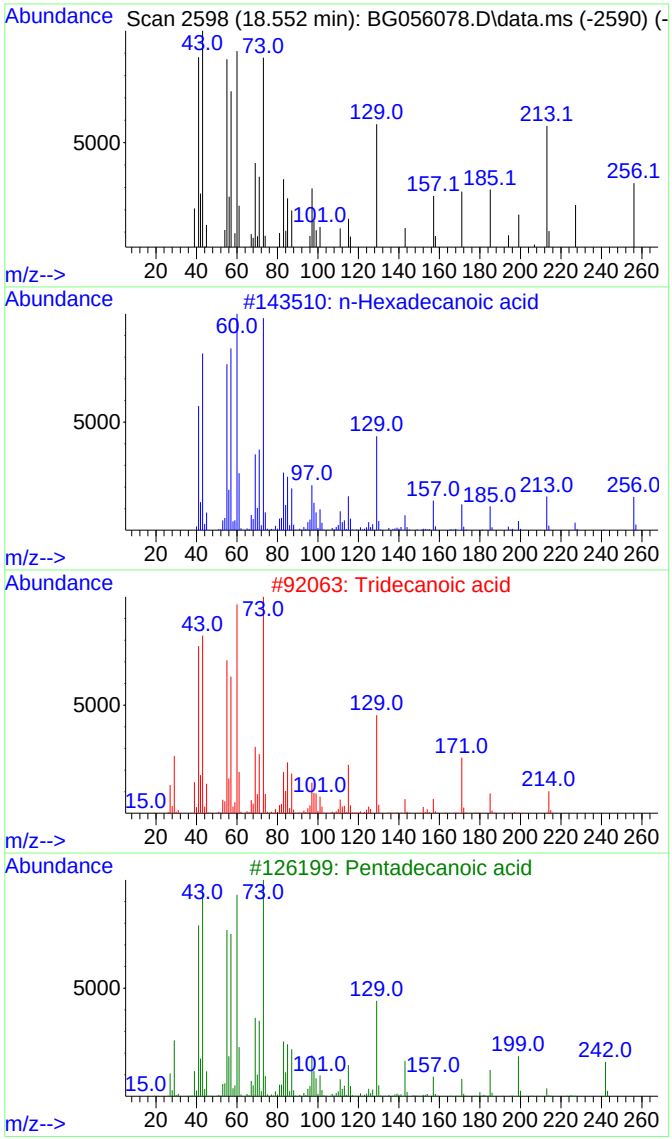
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

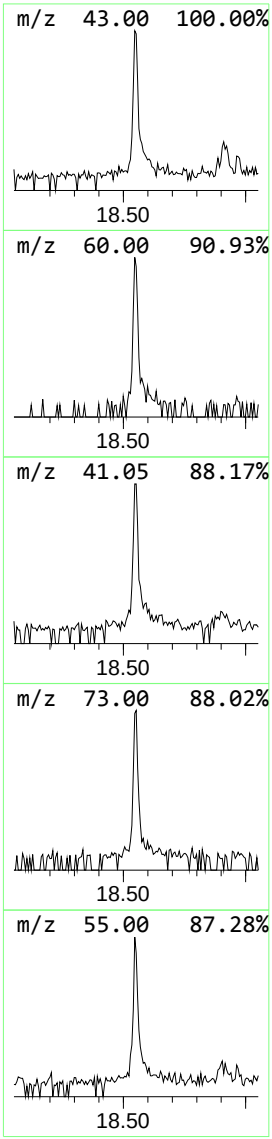
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.552	4.61 ng	39767	Phenanthrene-d10	17.700

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	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





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Sample : N6157-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221419-COMPOSITE-B

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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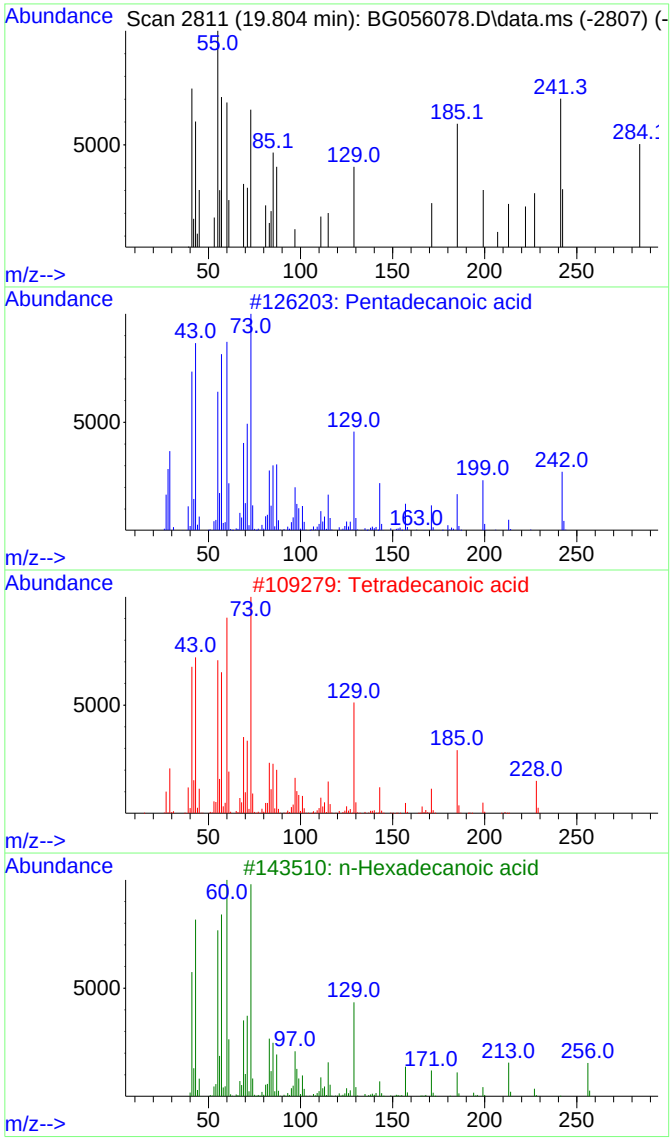
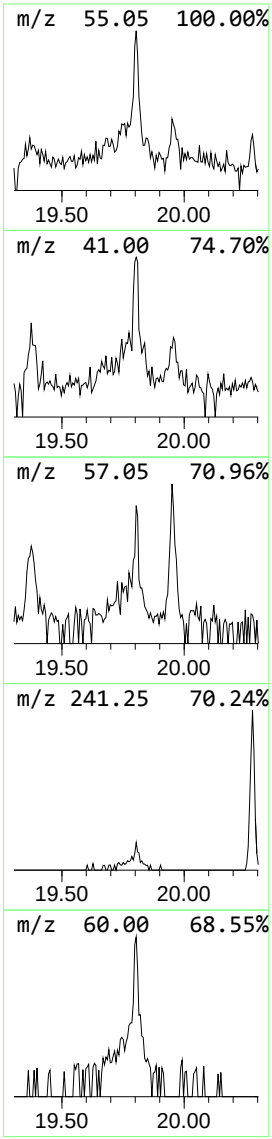
****

Peak Number 4 unknown19.804 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.804	2.84 ng	24529	Phenanthrene-d10	17.700

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	22
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	14
4	Tridecanoic acid	214	C13H26O2	000638-53-9	14
5	.alpha.-D-Galactopyranoside, met...	432	C21H36O9	1000157-03-2	12





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221419-COMPOSITE-B

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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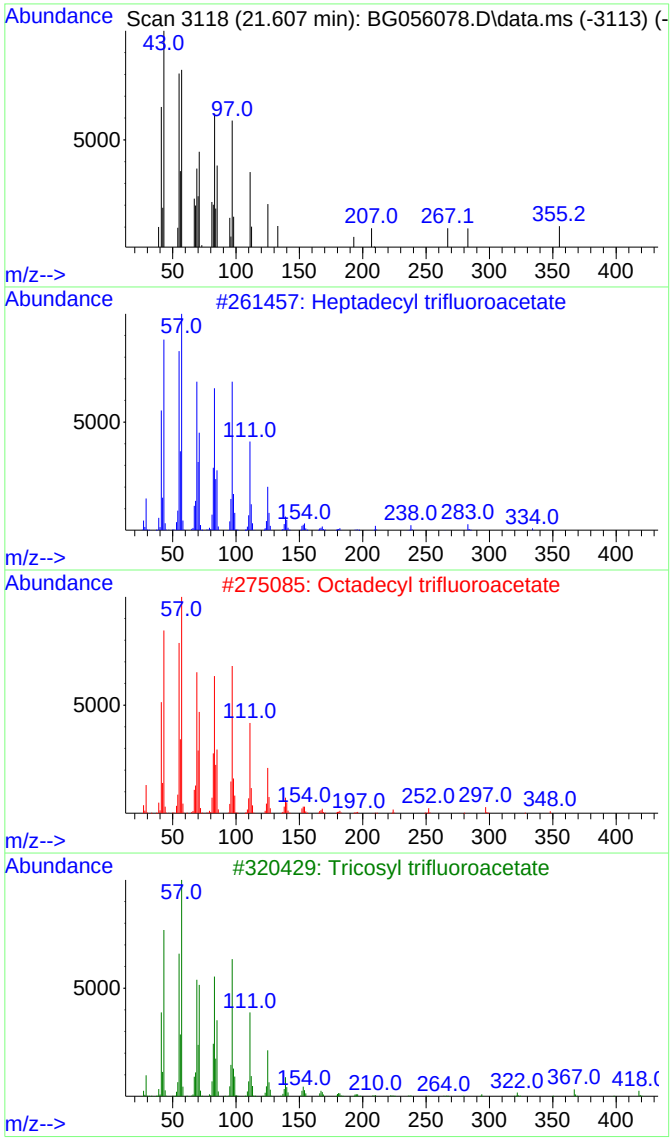
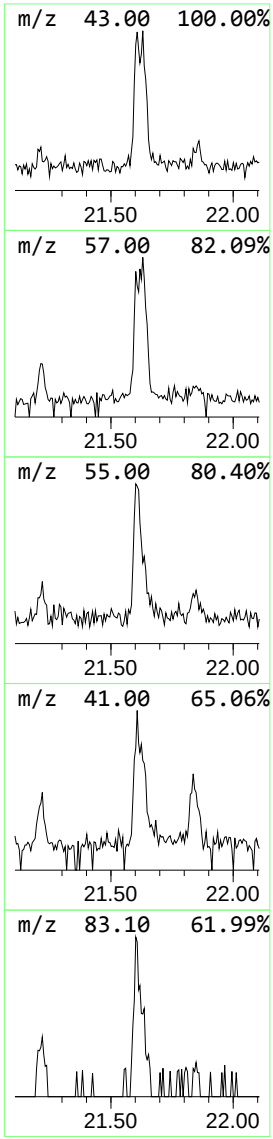
****

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.607	3.40 ng	40143	Chrysene-d12	22.013

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	76
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	76
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	74
4	17-Pentatriacontene	491	C35H70	006971-40-0	74
5	Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	74





Tentatively Identified Compound (LSC) summary

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BNA_G
ClientSampleId :
20221419-COMPOSITE-B

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.382	15.4	ng	37185	1	8.358	48217	20.0
2-Pentanone, 4-...	5.397	30.4	ng	73164	1	8.358	48217	20.0
n-Hexadecanoic ...	18.552	4.6	ng	39767	4	17.700	172481	20.0
unknown19.804	19.804	2.8	ng	24529	4	17.700	172481	20.0
Heptadecyl trif...	21.607	3.4	ng	40143	5	22.013	236132	20.0