LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056001.D
Acq On : 16 Dec 2022 19:52
Operator : CG/JU
Sample : N6038-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-40-(3-5)

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: BG056001.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	15	19	32	rBV	13222	22249	3.64%	0.763%
2	5.415	357	362	368	rBV	12426	18265	2.99%	0.627%
3	5.891	437	443	450	rBB	79136	126086	20.62%	4.325%
4	7.501	710	717	724	rBB	81918	138920	22.72%	4.766%
5	8.370	859	865	871	rBB	26903	42745	6.99%	1.466%
6	9.546	1057	1065	1071	rBB	48402	85607	14.00%	2.937%
7	11.202	1341	1347	1354	rBB	34201	59433	9.72%	2.039%
8	13.606	1750	1756	1763	rBB	182150	268462	43.91%	9.210%
9	14.980	1983	1990	1996	rBB	67574	103294	16.90%	3.544%
10	16.314	2212	2217	2223	rBV	31343	44984	7.36%	1.543%
11	16.455	2235	2241	2248	rVB	233949	347084	56.77%	11.907%
12	17.718	2449	2456	2461	rBV	107312	163788	26.79%	5.619%
13	18.564	2595	2600	2608	rBV3	24325	34167	5.59%	1.172%
14	18.776	2632	2636	2640	rBV5	3223	6709	1.10%	0.230%
15	19.745	2795	2801	2808	rVB	29055	39729	6.50%	1.363%
16	19.816	2810	2813	2820	rVB5	5719	8082	1.32%	0.277%
17	20.069	2852	2856	2858	rBV	5917	8404	1.37%	0.288%
18	20.104	2858	2862	2868	rVB	29681	43079	7.05%	1.478%
19	20.292	2888	2894	2899	rBV	485040	611338	100.00%	20.972%
20	20.415	2910	2915	2918	rBV6	4885	8821	1.44%	0.303%
21	20.591	2940	2945	2949	rVB2	7435	12254	2.00%	0.420%
22	20.691	2956	2962	2965	rBV2	4887	8297	1.36%	0.285%
23	20.750	2965	2972	2975	rBV6	4951	11752	1.92%	0.403%
24	20.832	2980	2986	2991	rVV9	4820	11128	1.82%	0.382%
25	21.614	3114	3119	3125	rVB4	20624	32060	5.24%	1.100%
26	21.884	3160	3165	3169	rBV2	11191	17140	2.80%	0.588%
27	22.025	3180	3189	3194	rBV3	118893	244766	40.04%	8.397%
28	22.072	3194	3197	3203	rVB	16791	27748	4.54%	0.952%
29	22.877	3330	3334	3340	rVB7	7192	16328	2.67%	0.560%
30	23.841	3494	3498	3504	rVB6	9595	17690	2.89%	0.607%
31	24.405	3585	3594	3598	rBV4	16866	48804	7.98%	1.674%
32	25.192	3723	3728	3729	rBV3	4543	6971	1.14%	0.239%
33	25.351	3749	3755	3767	rVB2	11393	36086	5.90%	1.238%
34	25.521	3775	3784	3797	rBV2	72620	220663	36.10%	7.570%
35	26.808	3996	4003	4013	rVB9	6578	22045	3.61%	0.756%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056001.D
Acq On : 16 Dec 2022 19:52
Operator : CG/JU
Sample : N6038-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-40-(3-5)

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

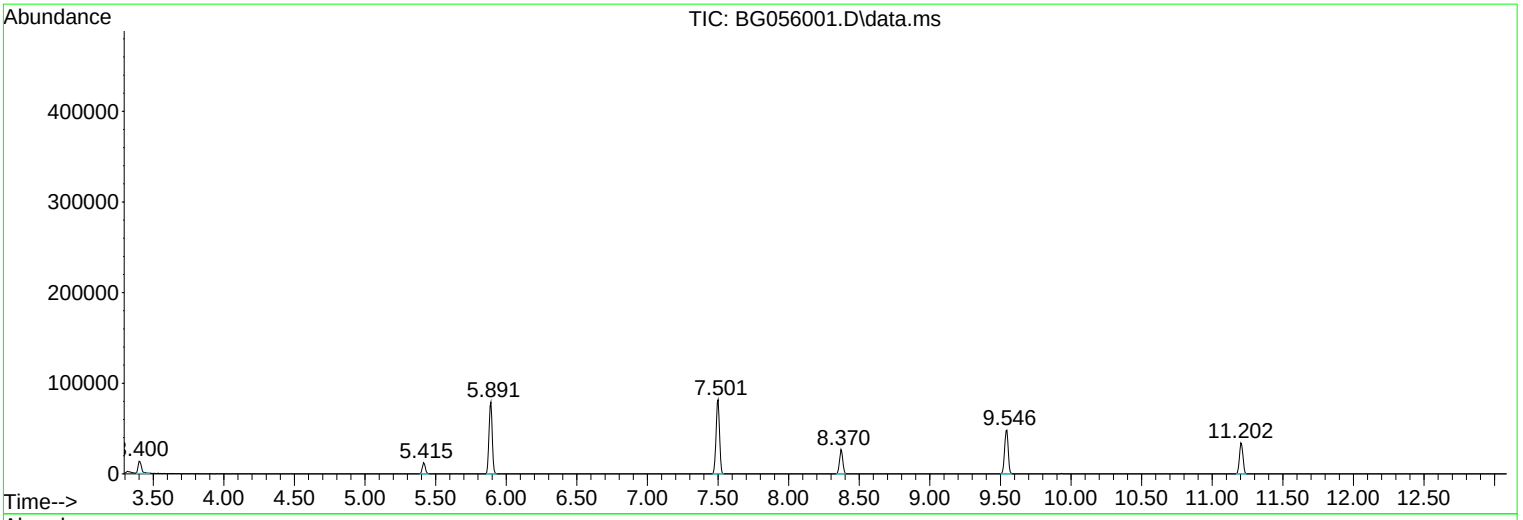
Sum of corrected areas: 2914978

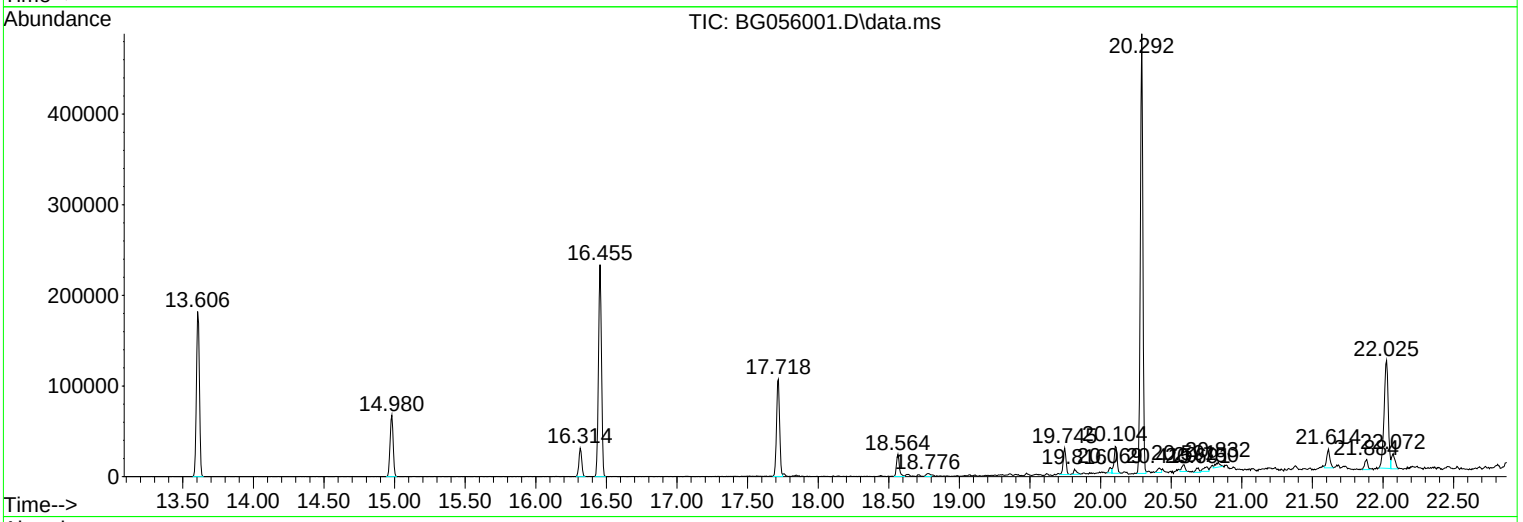
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056001.D
Acq On : 16 Dec 2022 19:52
Operator : CG/JU
Sample : N6038-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

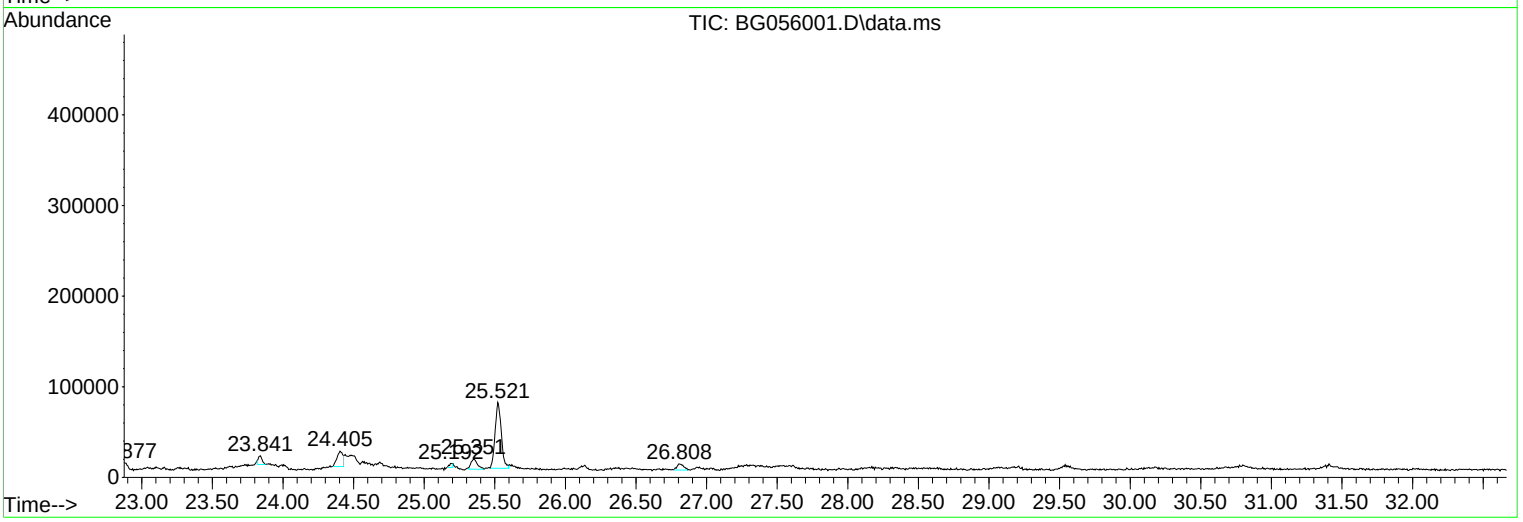
Instrument :
BNA_G
ClientSampleId :
RB-40-(3-5)

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\BG121622\
Data File : BG056001.D
Acq On : 16 Dec 2022 19:52
Operator : CG/JU
Sample : N6038-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-40-(3-5)

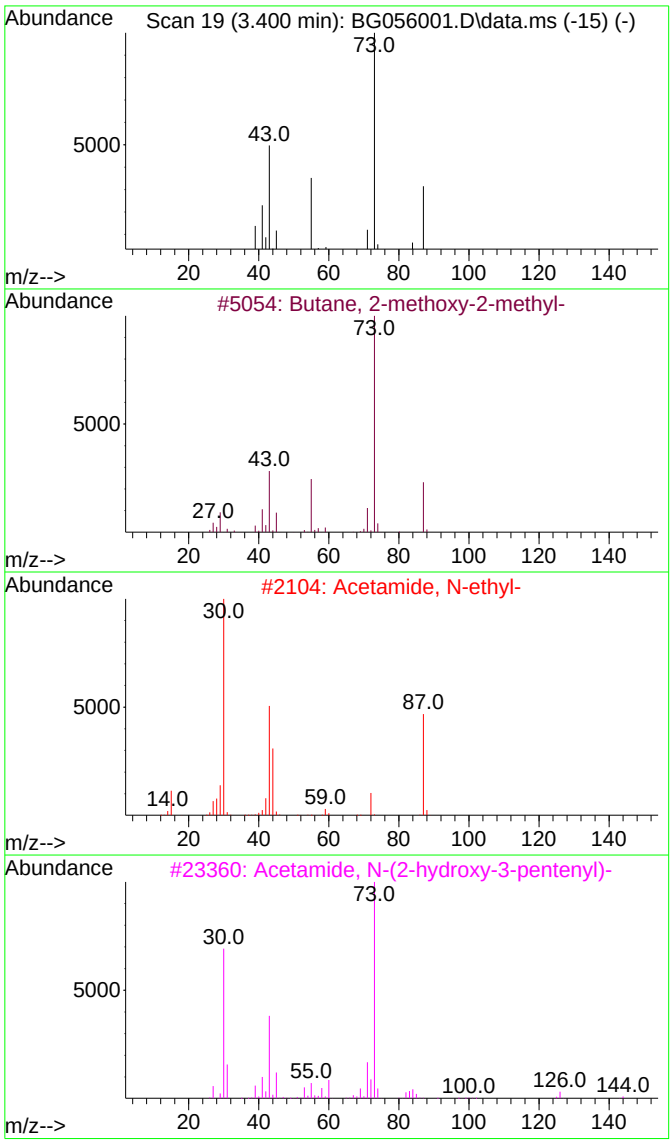
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

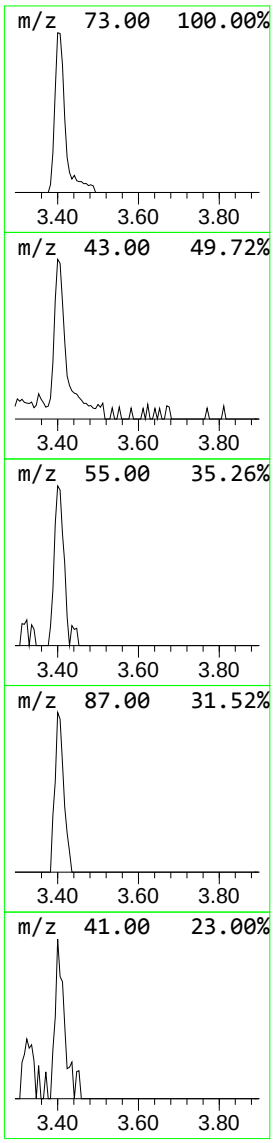
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.400	10.41 ng	22249	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	83
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3	Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	9
4	2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	9
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056001.D
Acq On : 16 Dec 2022 19:52
Operator : CG/JU
Sample : N6038-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-40-(3-5)

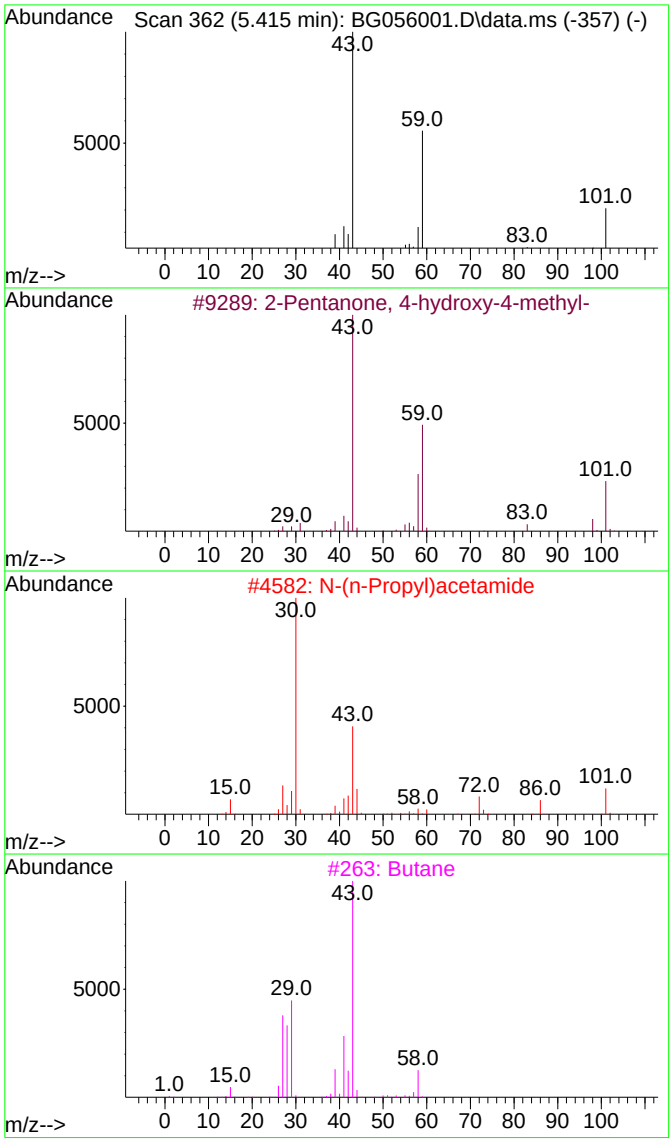
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

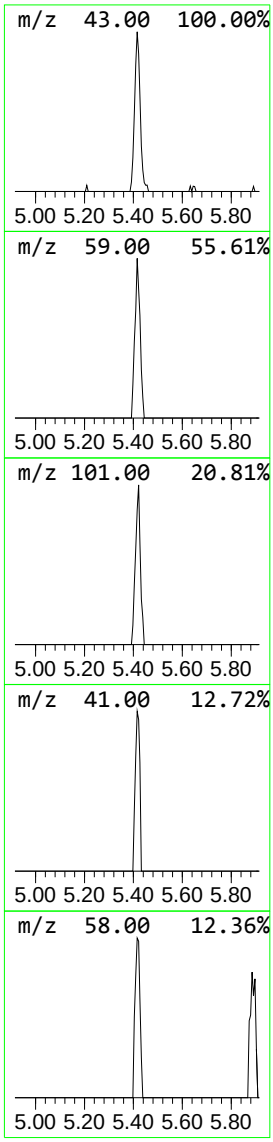
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.415	8.55 ng	18265	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	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9
3	Butane	58	C4H10	000106-97-8	9
4	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056001.D
Acq On : 16 Dec 2022 19:52
Operator : CG/JU
Sample : N6038-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-40-(3-5)

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

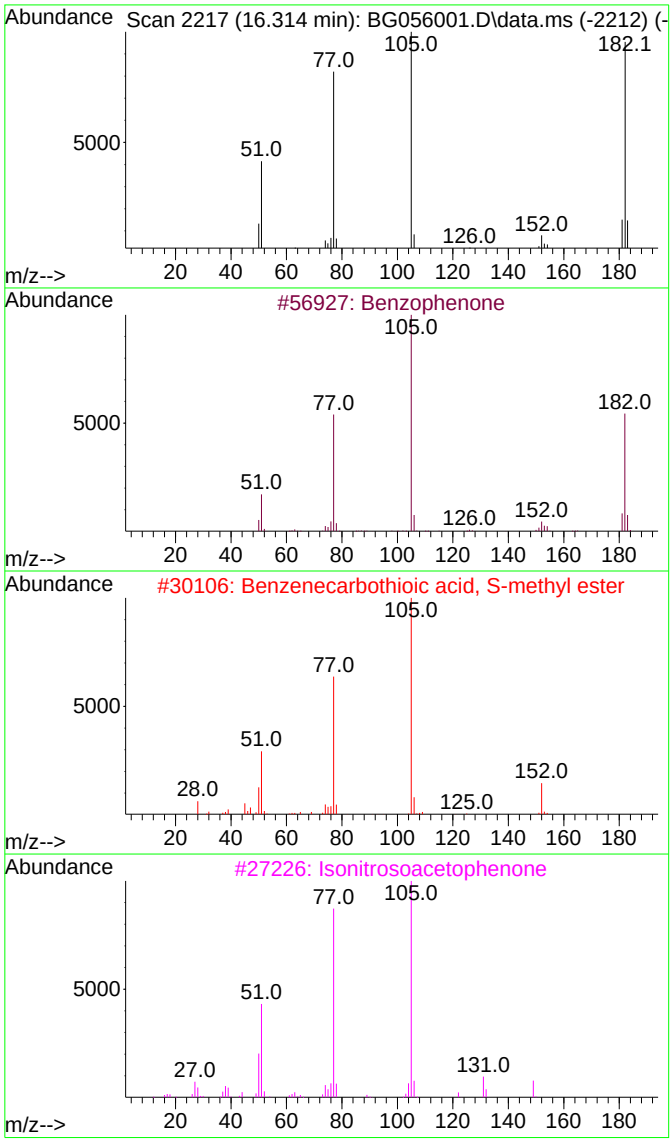
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

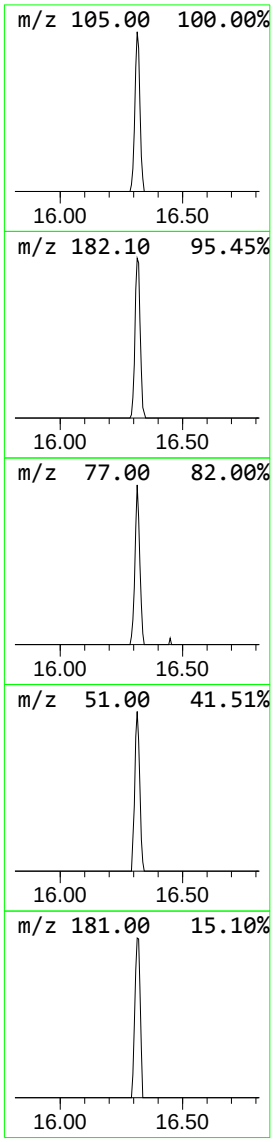
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.314	8.71 ng	44984	Acenaphthene-d10	14.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3	Isonitrosoacetophenone	149	C8H7NO2	000532-54-7	43
4	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	43
5	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056001.D
Acq On : 16 Dec 2022 19:52
Operator : CG/JU
Sample : N6038-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-40-(3-5)

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

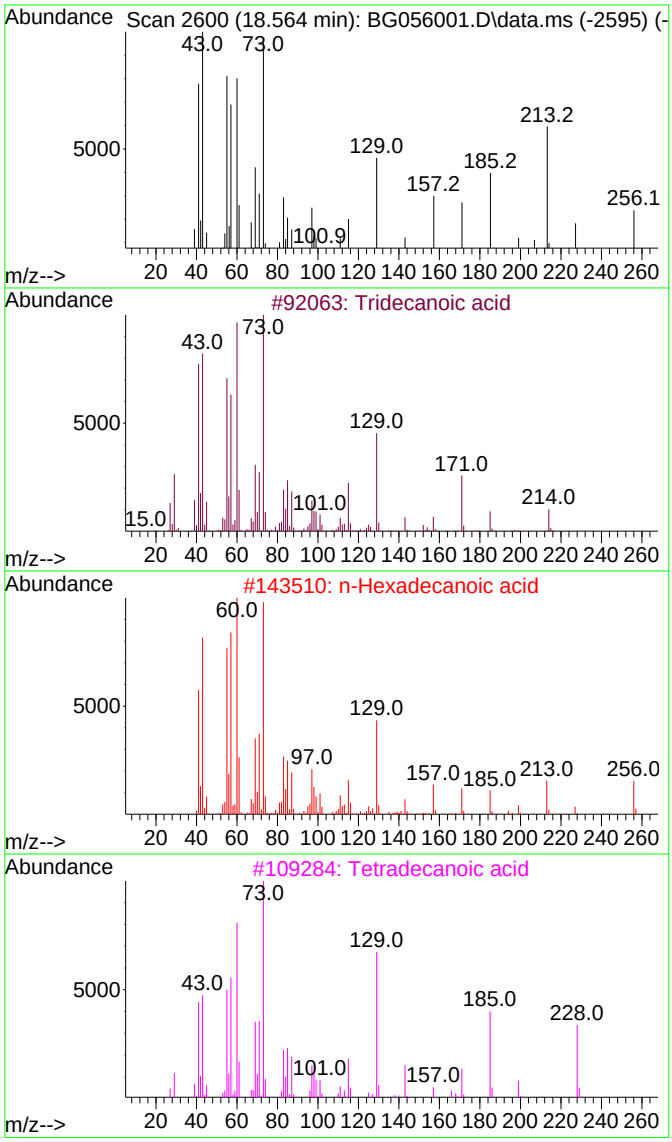
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

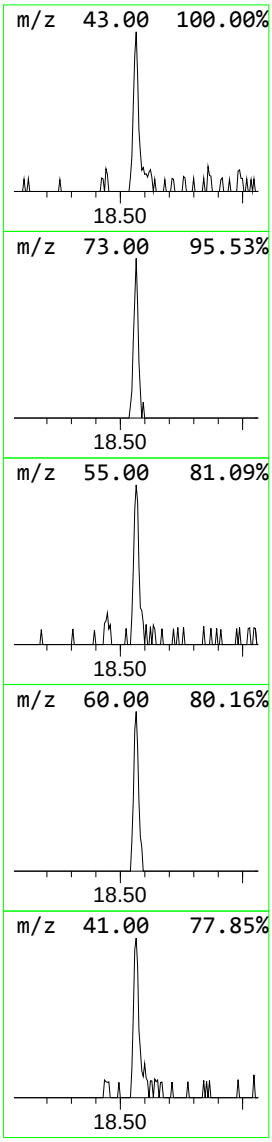
****

Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.564	4.17 ng	34167	Phenanthrene-d10	17.718

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	52
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
5	n-Decanoic acid	172	C10H20O2	000334-48-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056001.D
Acq On : 16 Dec 2022 19:52
Operator : CG/JU
Sample : N6038-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-40-(3-5)

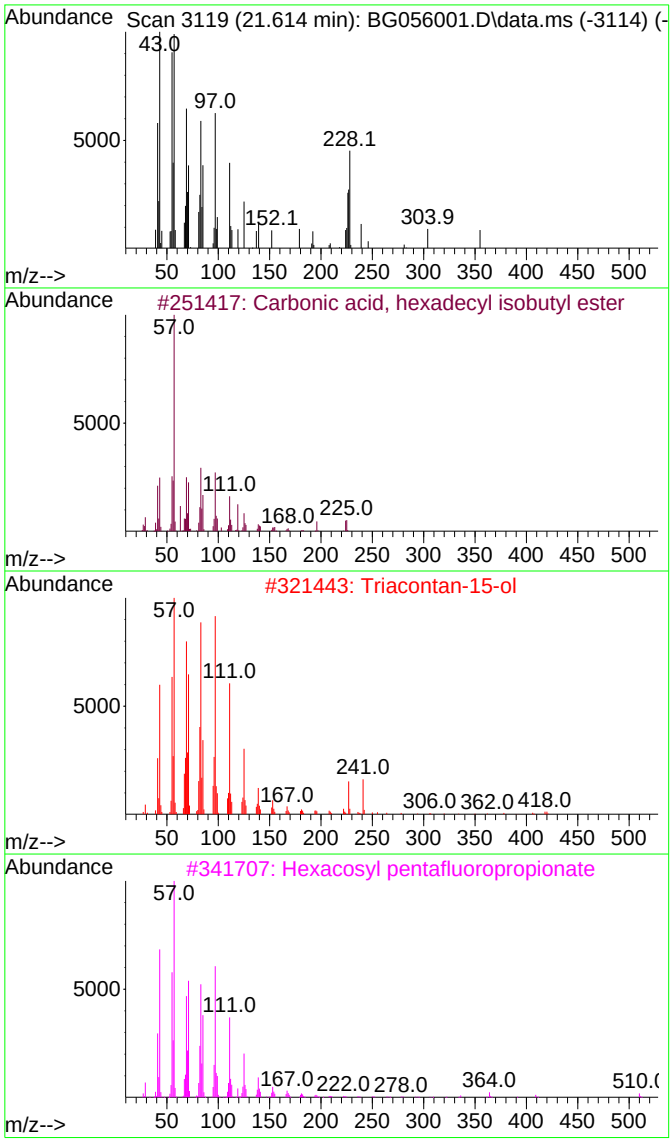
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

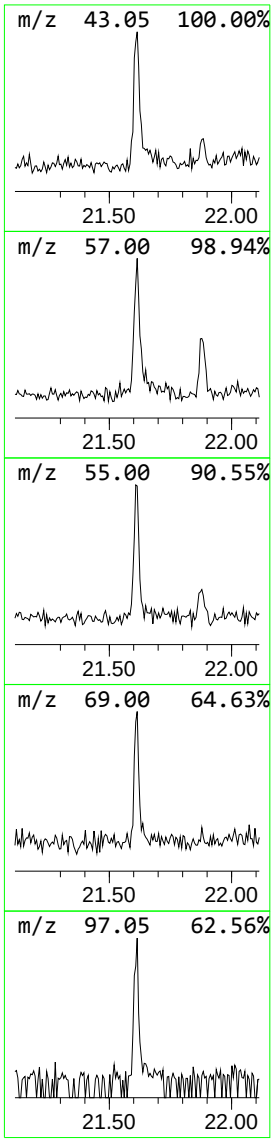
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Carbonic acid, hexadecyl is... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.614	2.62 ng	32060	Chrysene-d12	22.025

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl isobuty...	342	C21H42O3	1010314-61-3	58
2	Triacontan-15-ol	438	C30H62O	031849-26-0	53
3	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	52
4	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	52
5	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056001.D
Acq On : 16 Dec 2022 19:52
Operator : CG/JU
Sample : N6038-23
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-40-(3-5)

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...	3.400	10.4	ng	22249	1	8.370	42745	20.0
2-Pentanone, 4-...	5.415	8.6	ng	18265	1	8.370	42745	20.0
Benzophenone	16.314	8.7	ng	44984	3	14.980	103294	20.0
Tridecanoic acid	18.564	4.2	ng	34167	4	17.718	163788	20.0
Carbonic acid, ...	21.614	2.6	ng	32060	5	22.025	244766	20.0