LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(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: BG056002.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	13	19	26	rBV	18702	29580	4.02%	0.831%
2	5.414	357	362	368	rBB	17192	24905	3.38%	0.700%
3	5.890	436	443	449	rBB	97495	152319	20.69%	4.280%
4	7.500	710	717	723	rBB	100687	166358	22.60%	4.675%
5	8.370	859	865	871	rBB	27637	46014	6.25%	1.293%
6	9.545	1057	1065	1072	rBB	58102	104263	14.16%	2.930%
7	11.207	1341	1348	1355	rBB	36693	64049	8.70%	1.800%
8	13.611	1750	1757	1763	rBB	212312	326411	44.34%	9.173%
9	14.980	1984	1990	1997	rBB2	72729	110067	14.95%	3.093%
10	16.313	2212	2217	2223	rBB	27638	38109	5.18%	1.071%
11	16.454	2235	2241	2250	rBB	282039	427226	58.04%	12.006%
12	17.717	2449	2456	2460	rBV	116664	175022	23.78%	4.918%
13	17.759	2460	2463	2468	rVB	14243	19010	2.58%	0.534%
14	18.564	2595	2600	2607	rBV3	26496	36933	5.02%	1.038%
15	18.781	2631	2637	2640	rBV3	3829	7677	1.04%	0.216%
16	19.745	2796	2801	2807	rVB	58810	81911	11.13%	2.302%
17	19.815	2808	2813	2821	rBV5	5199	8427	1.14%	0.237%
18	20.074	2849	2857	2858	rBV	8135	12945	1.76%	0.364%
19	20.103	2858	2862	2869	rVB	46513	70011	9.51%	1.967%
20	20.291	2888	2894	2899	rBV	555898	736115	100.00%	20.686%
21	20.585	2939	2944	2949	rVB	9838	19164	2.60%	0.539%
22	20.685	2954	2961	2965	rBV2	6292	10967	1.49%	0.308%
23	20.749	2965	2972	2976	rVB3	5533	11656	1.58%	0.328%
24	21.372	3074	3078	3084	rVB3	5313	9643	1.31%	0.271%
25	21.613	3114	3119	3124	rVB4	27282	39986	5.43%	1.124%
26	21.672	3126	3129	3134	rVB3	5710	11386	1.55%	0.320%
27	21.730	3134	3139	3144	rVB2	5762	9239	1.26%	0.260%
28	22.024	3180	3189	3195	rBV3	127210	283949	38.57%	7.980%
29	22.071	3195	3197	3205	rVB	28441	41509	5.64%	1.166%
30	22.453	3258	3262	3268	rBV6	4398	9188	1.25%	0.258%
31	22.876	3328	3334	3341	rVB10	9313	22936	3.12%	0.645%
32	23.834	3493	3497	3505	rVB7	6665	12309	1.67%	0.346%
33	24.398	3585	3593	3601	rBV2	23451	80902	10.99%	2.274%
34	25.197	3720	3729	3735	rBV2	14310	39221	5.33%	1.102%
35	25.356	3743	3756	3765	rBV	19248	60269	8.19%	1.694%
36	25.526	3774	3785	3796	rBV3	75148	231073	31.39%	6.494%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(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

37	26.819	3998	4005	4014	rVB10	5709	18709	2.54%	0.526%
38	29.533	4461	4467	4468	rBV3	5110	9016	1.22%	0.253%

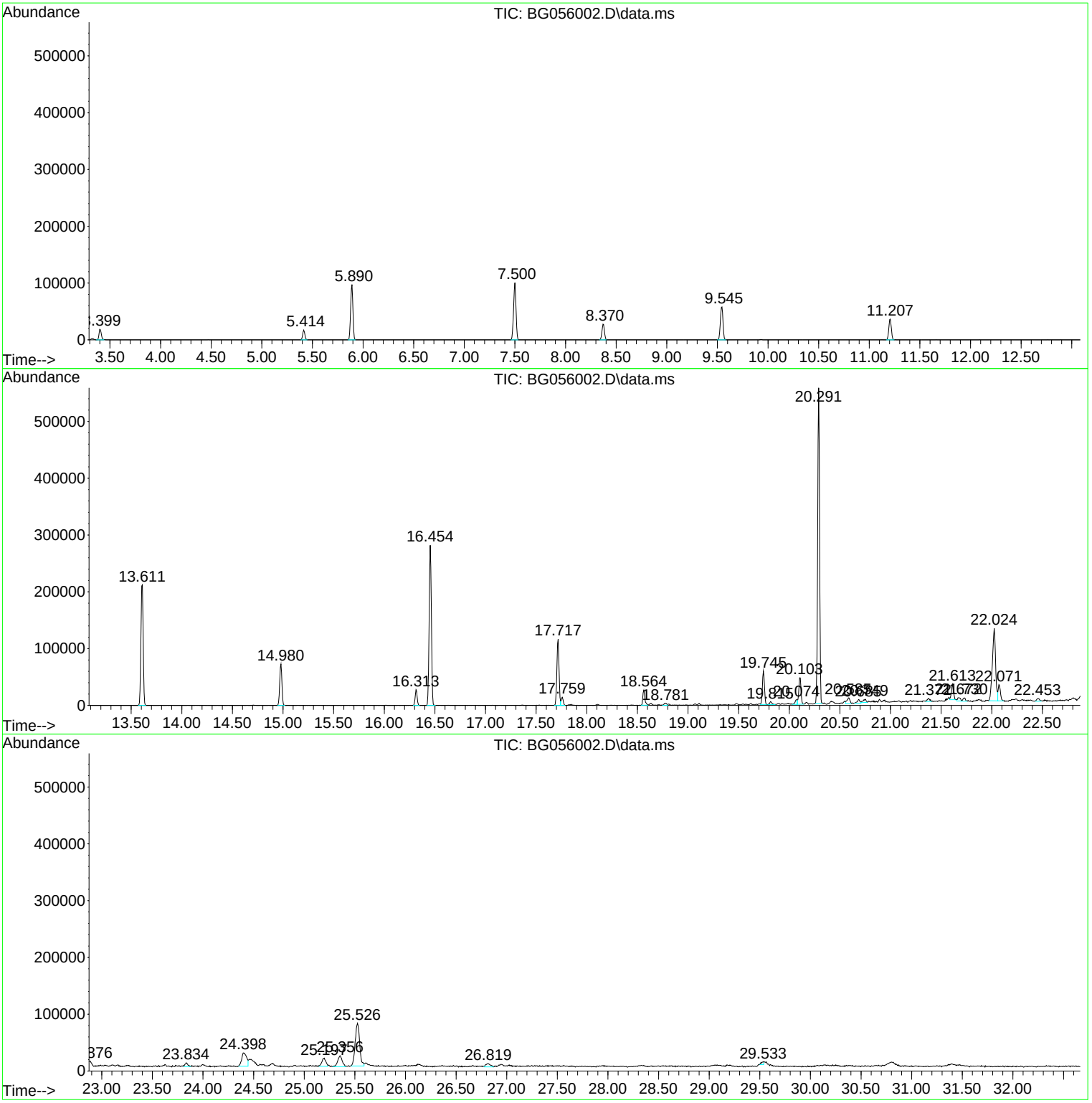
Sum of corrected areas: 3558474

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(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 : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(3-5)

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

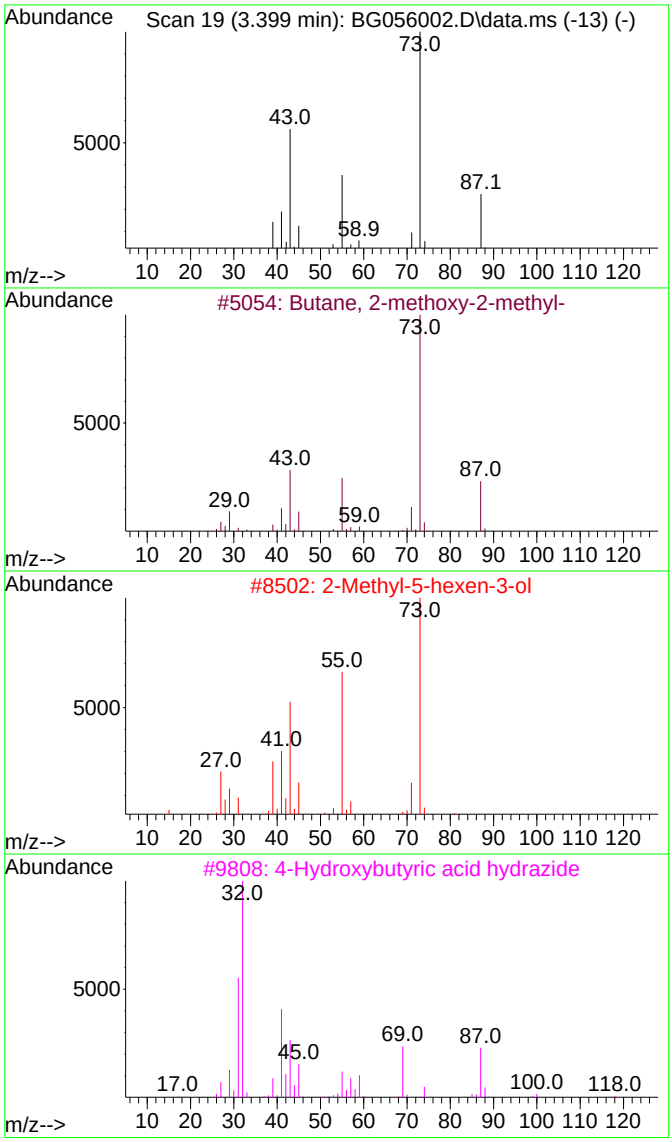
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

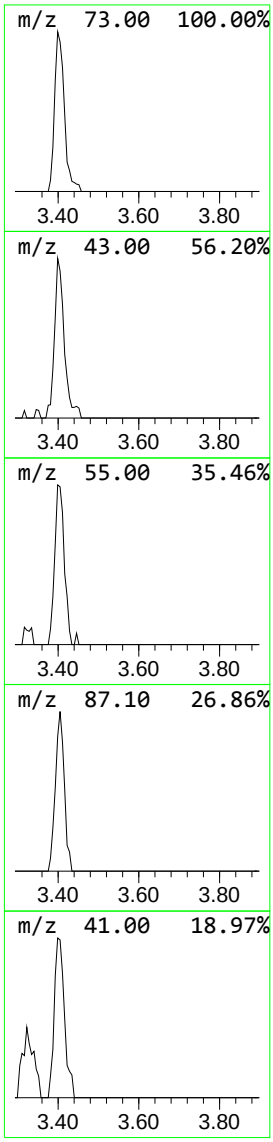
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	12.86 ng	29580	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	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3	4-Hydroxybutyric acid hydrazide	118	C4H10N2O2	003879-08-1	12
4	(R)-3-Pyrrolidinol	87	C4H9NO	002799-21-5	9
5	1,2-Propanediol, 2-acetate	118	C5H10O3	006214-01-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(3-5)

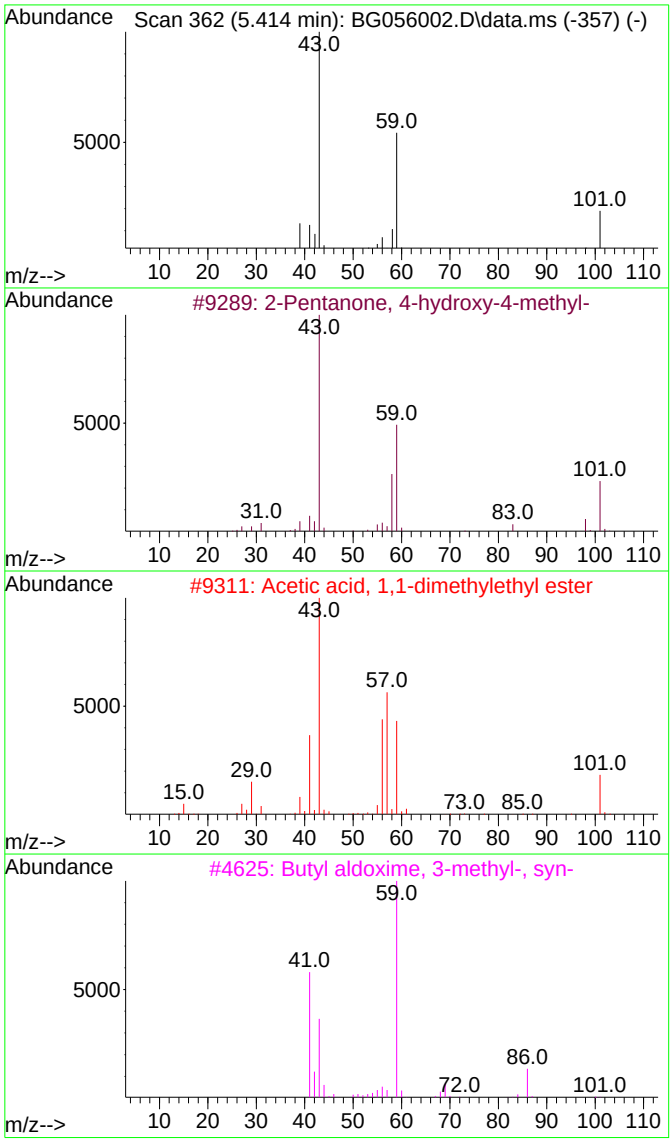
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

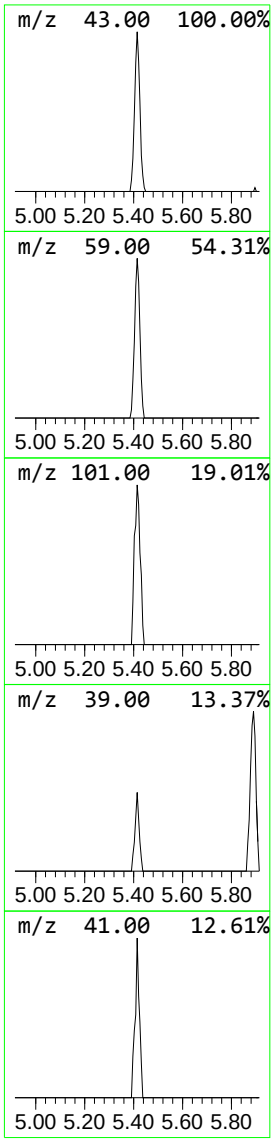
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.414	10.82 ng	24905	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	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	40
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	Butane	58	C4H10	000106-97-8	12
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(3-5)

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

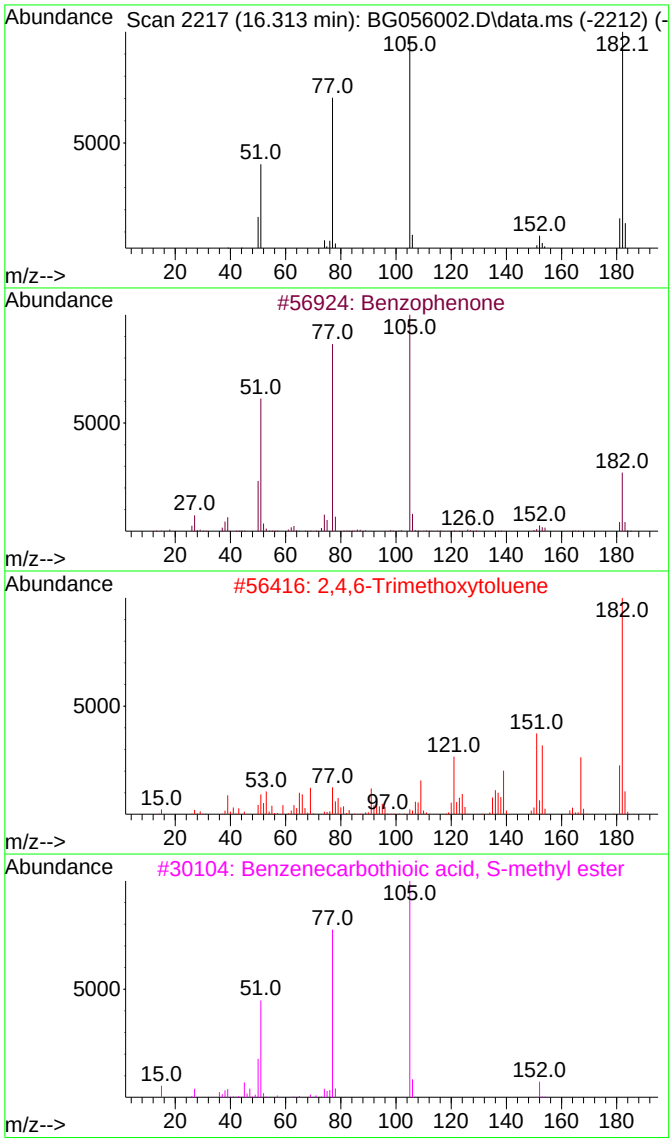
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

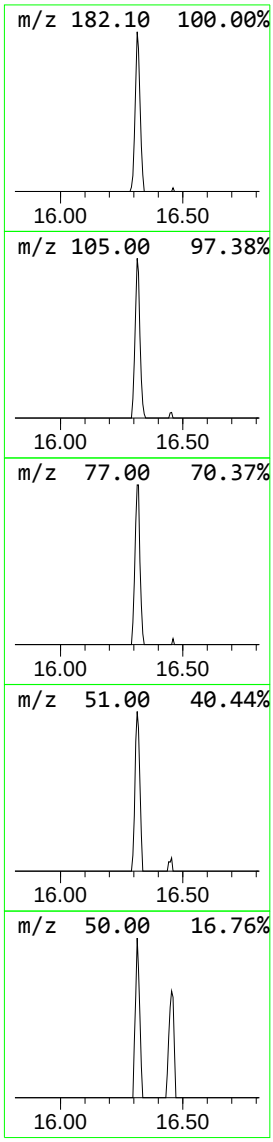
****

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.313	6.92 ng	38109	Acenaphthene-d10	14.980

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	41
4	7-Phosphabicyclo[2.2.1]hept-2-en...	182	C11H19P	1000151-83-5	38
5	3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(3-5)

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

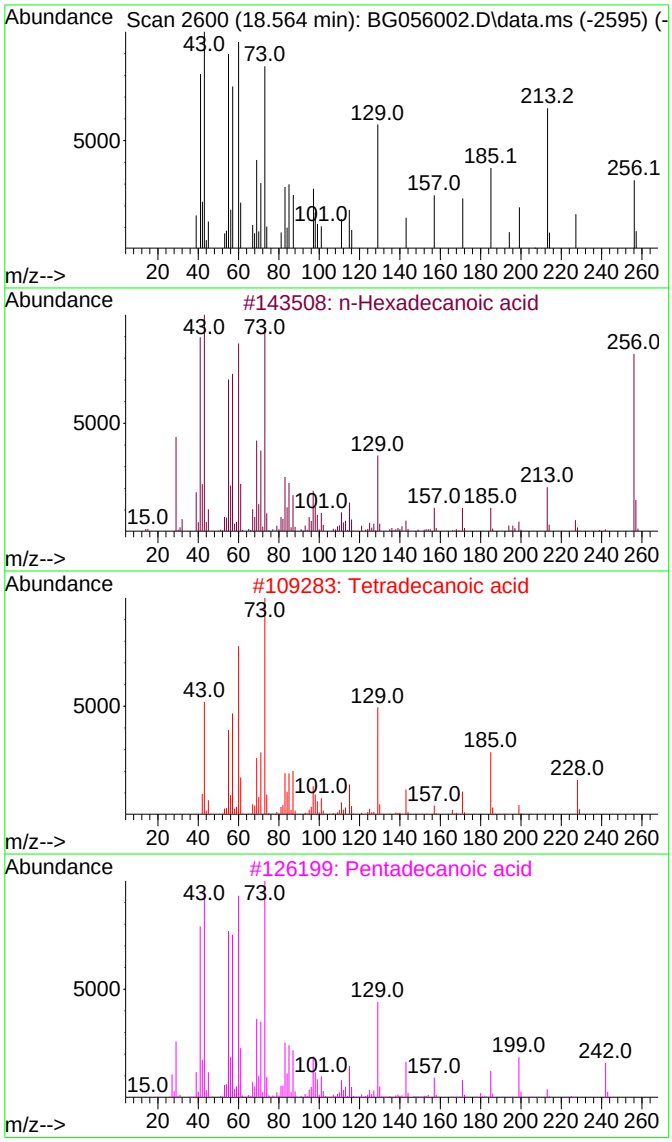
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

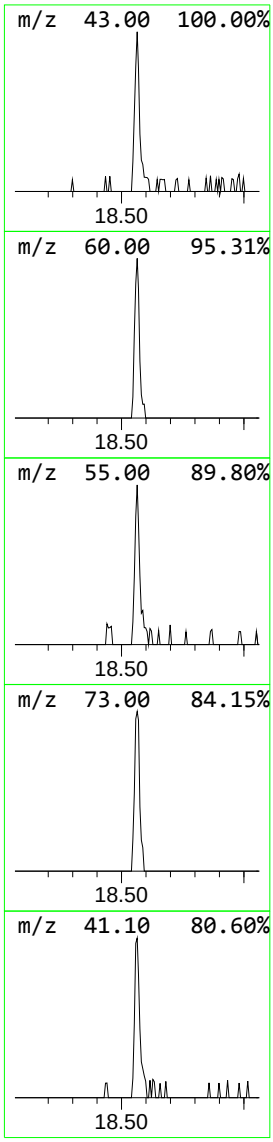
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.564	4.22 ng	36933	Phenanthrene-d10	17.718

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	Tridecanoic acid	214	C13H26O2	000638-53-9	46
5	n-Decanoic acid	172	C10H20O2	000334-48-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(3-5)

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

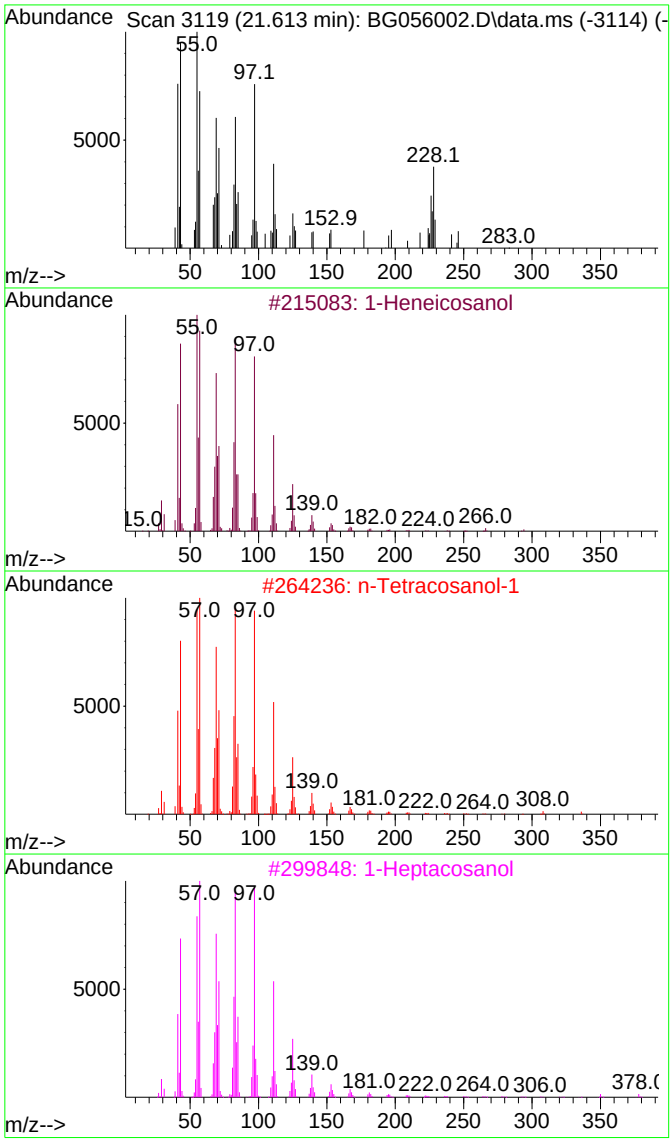
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

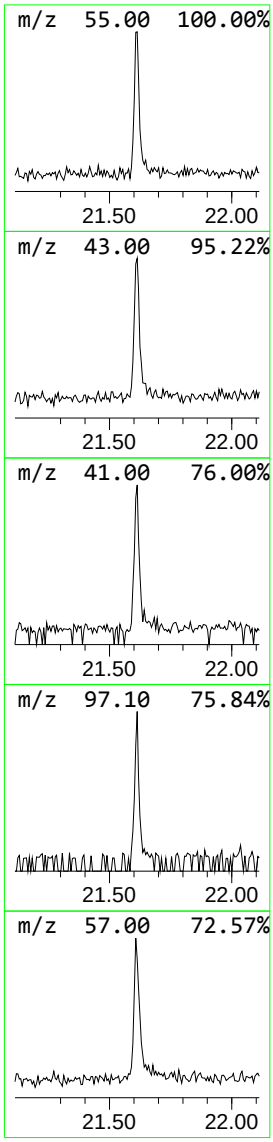
****

Peak Number 5 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.613	2.82 ng	39986	Chrysene-d12	22.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	1-Hexacosanol	382	C26H54O	000506-52-5	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(3-5)

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

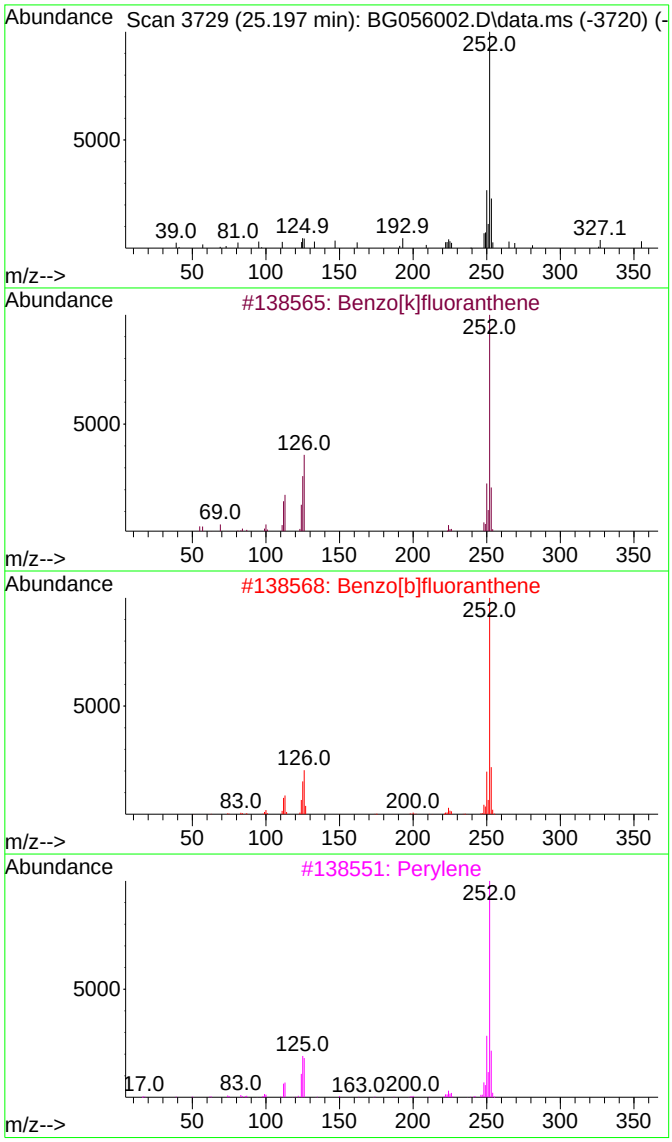
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

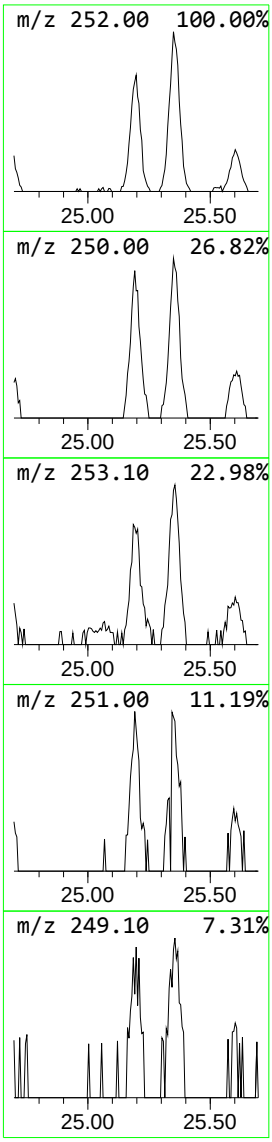
****

Peak Number 6 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.197	3.39 ng	39221	Perylene-d12	25.526

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
3	Perylene	252	C20H12	000198-55-0	76
4	Benzo[e]pyrene	252	C20H12	000192-97-2	74
5	Benzo[a]pyrene	252	C20H12	000050-32-8	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
Data File : BG056002.D
Acq On : 16 Dec 2022 20:33
Operator : CG/JU
Sample : N6038-27
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RB-42-(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...	3.399	12.9	ng	29580	1	8.370	46014	20.0
2-Pentanone, 4-...	5.414	10.8	ng	24905	1	8.370	46014	20.0
Benzophenone	16.313	6.9	ng	38109	3	14.980	110067	20.0
n-Hexadecanoic ...	18.564	4.2	ng	36933	4	17.718	175022	20.0
1-Heneicosanol	21.613	2.8	ng	39986	5	22.024	283949	20.0
Perylene	25.197	3.4	ng	39221	6	25.526	231073	20.0