LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102618\
Data File : BG037587.D
Acq On : 26 Oct 2018 19:10
Operator : JU/SJ
Sample : J5649-10
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DL-04A

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-BG101818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.766	77	81	92	rBV	41944	72304	1.85%	0.327%
2	5.182	316	322	329	rBV	51944	87082	2.23%	0.393%
3	5.641	393	400	411	rBV	997053	1655950	42.33%	7.478%
4	7.245	663	673	688	rBV	1071716	2059611	52.65%	9.301%
5	7.627	730	738	748	rBV	993523	1750167	44.74%	7.903%
6	8.102	810	819	832	rVB	162363	288325	7.37%	1.302%
7	8.426	866	874	885	rVB	698248	1231213	31.47%	5.560%
8	9.278	1011	1019	1030	rBV	616868	1148079	29.35%	5.184%
9	10.923	1291	1299	1309	rVB	235313	439768	11.24%	1.986%
10	13.355	1704	1713	1725	rBV	1714654	2758514	70.51%	12.457%
11	14.178	1846	1853	1860	rBV	255359	378409	9.67%	1.709%
12	14.736	1939	1948	1956	rBV2	410161	681829	17.43%	3.079%
13	16.222	2193	2201	2218	rBV	1391321	2226620	56.92%	10.055%
14	17.480	2407	2415	2424	rBV	583454	896093	22.91%	4.047%
15	18.338	2556	2561	2569	rBV	92345	149402	3.82%	0.675%
16	19.601	2771	2776	2782	rBV3	39980	66243	1.69%	0.299%
17	20.083	2851	2858	2868	rBV	2808397	3912107	100.00%	17.666%
18	21.369	3072	3077	3091	rBV3	70777	159180	4.07%	0.719%
19	21.763	3137	3144	3154	rBV2	542495	924097	23.62%	4.173%
20	22.538	3271	3276	3281	rBV2	27000	48298	1.23%	0.218%
21	23.255	3393	3398	3405	rVB	37091	74815	1.91%	0.338%
22	24.084	3533	3539	3549	rVB2	38137	87321	2.23%	0.394%
23	25.100	3697	3712	3727	rBV2	270156	954068	24.39%	4.308%
24	26.234	3897	3905	3918	rVB4	27157	95001	2.43%	0.429%

Sum of corrected areas: 22144496

LSC Report - Integrated Chromatogram

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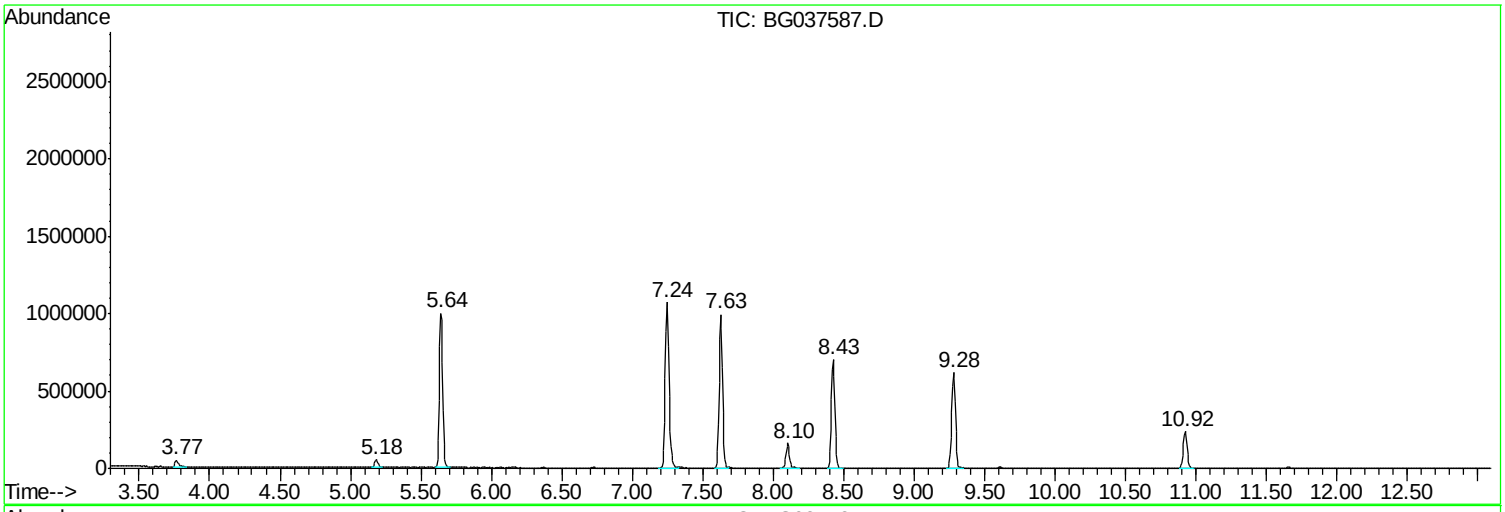
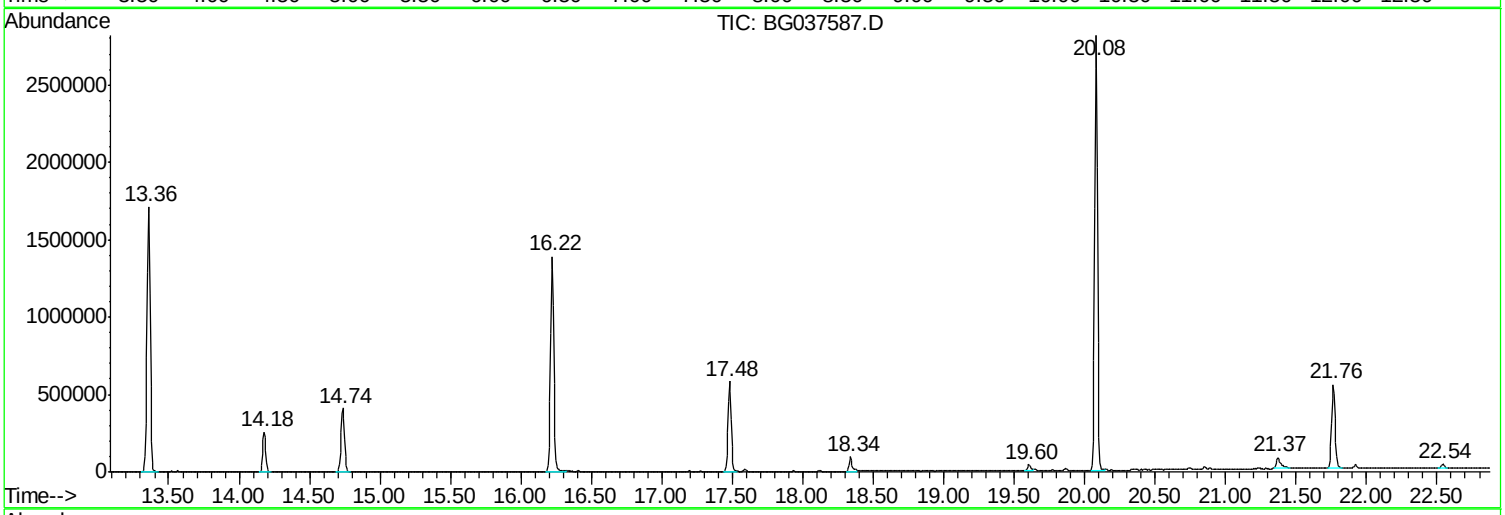
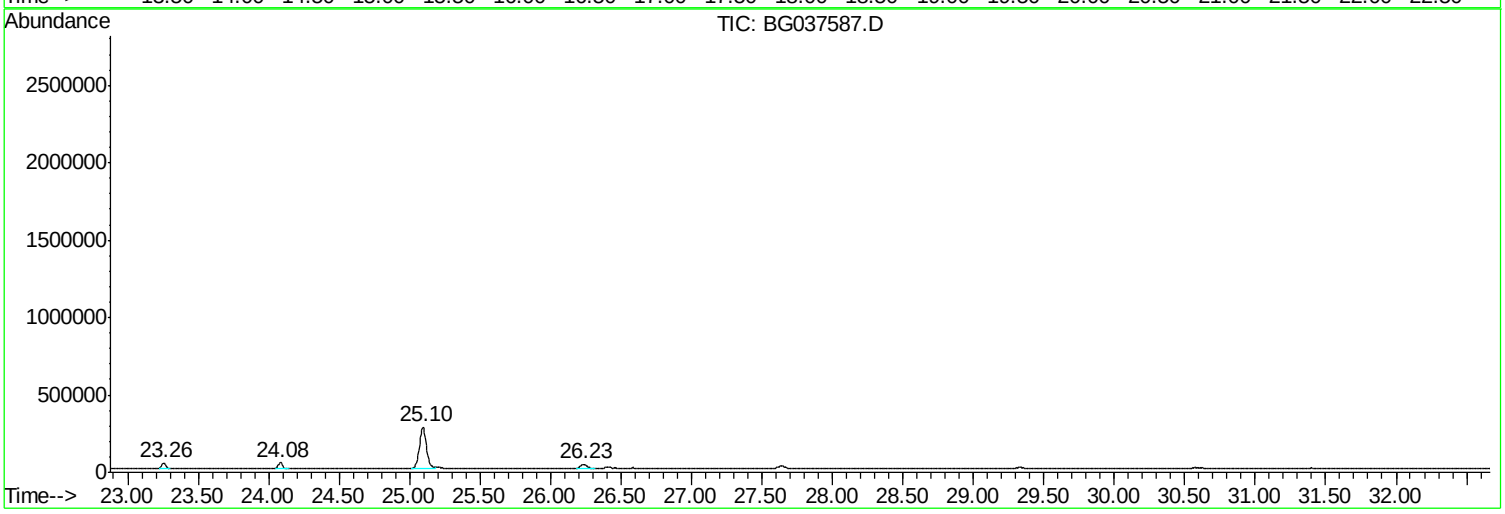
Instrument :
BNA_G
ClientSampleId :
DL-04A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P







Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

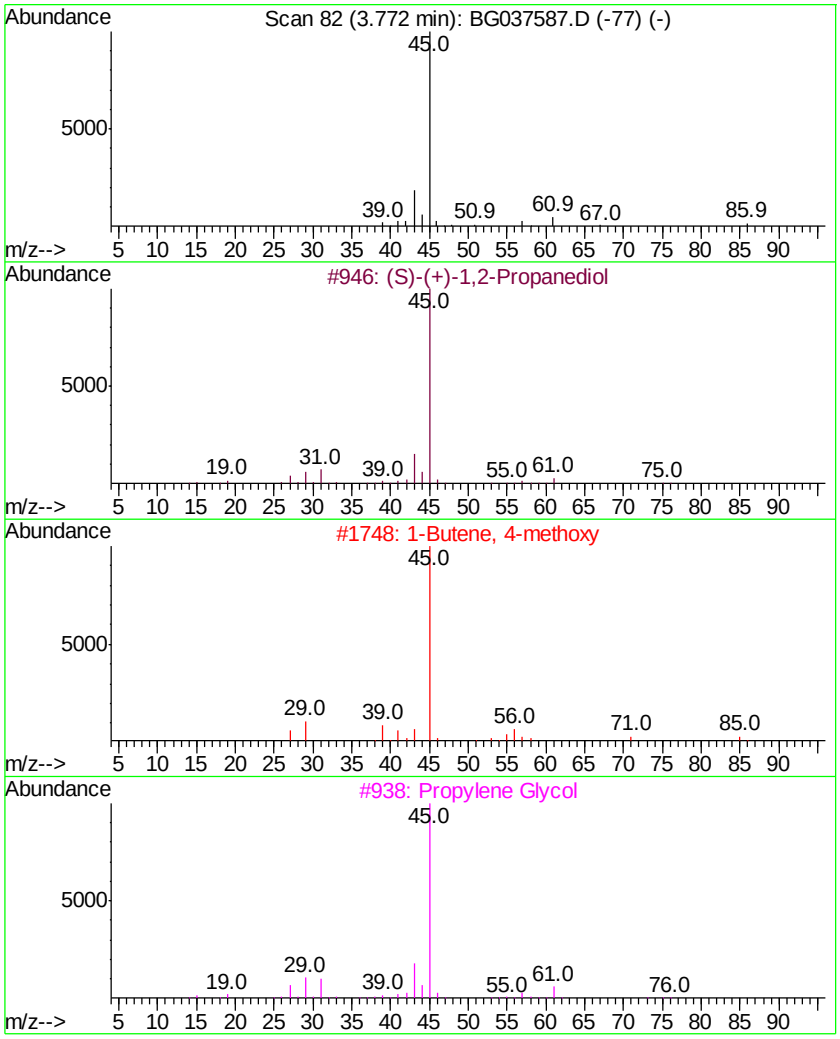
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

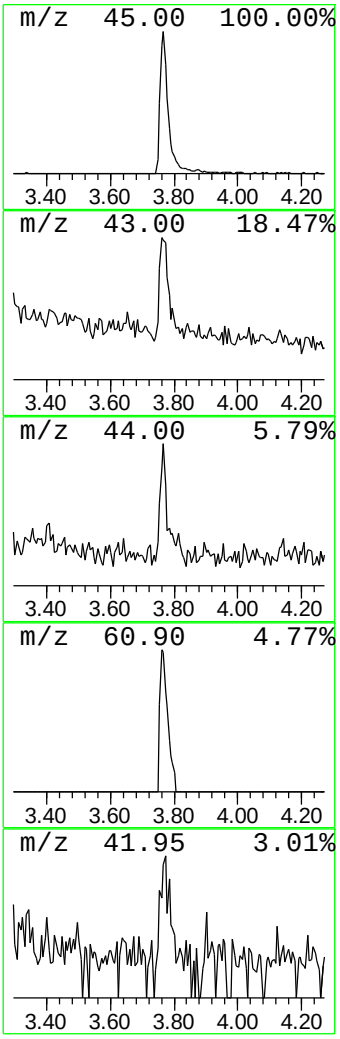
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.77	5.02 ng	72304	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	50
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	9
5	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9





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ALS Vial : 9 Sample Multiplier: 1

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

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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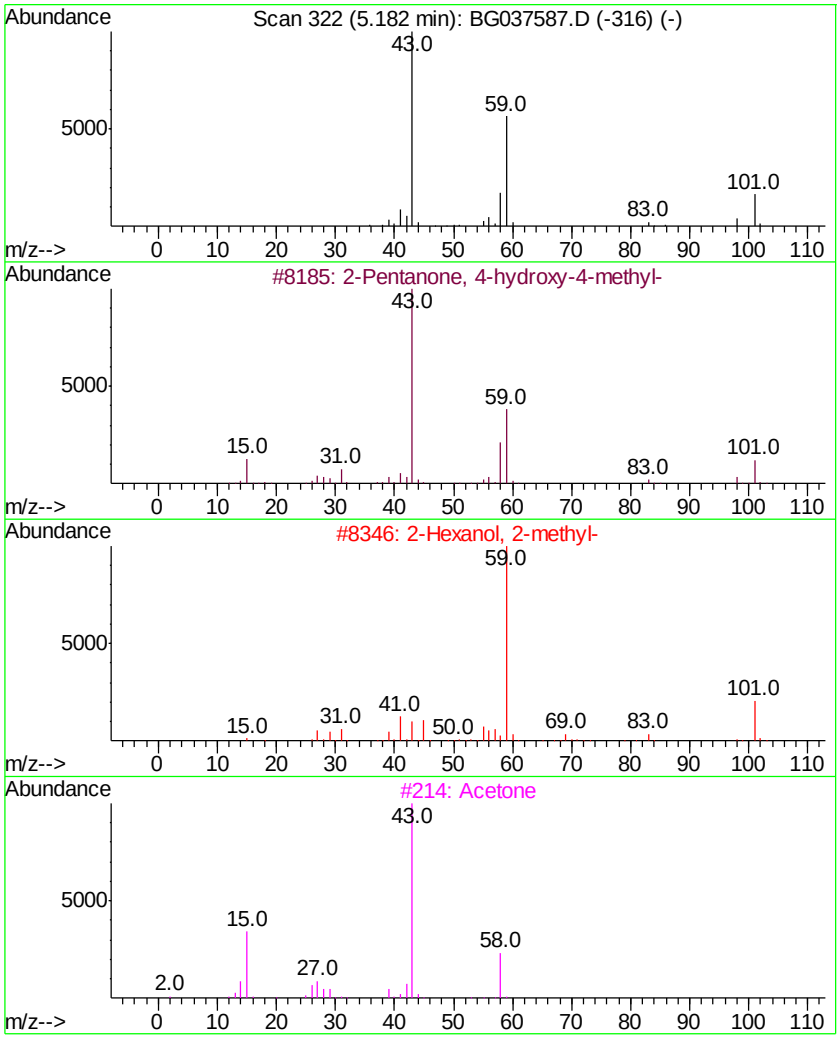
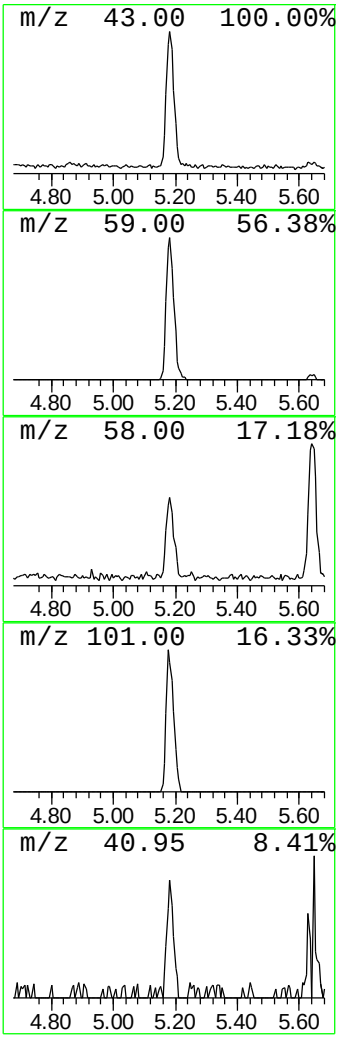
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	6.04 ng	87082	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	Acetone	58	C3H6O	000067-64-1	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Misc :
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Instrument :
BNA_G
ClientSampleId :
DL-04A

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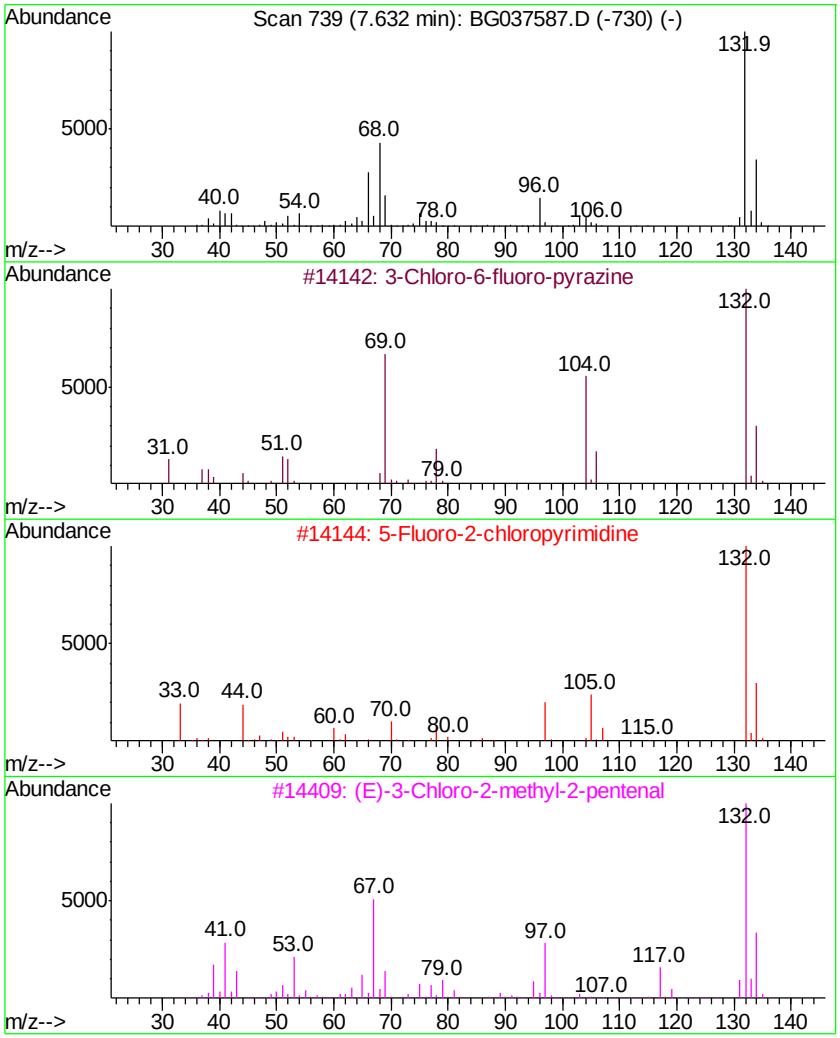
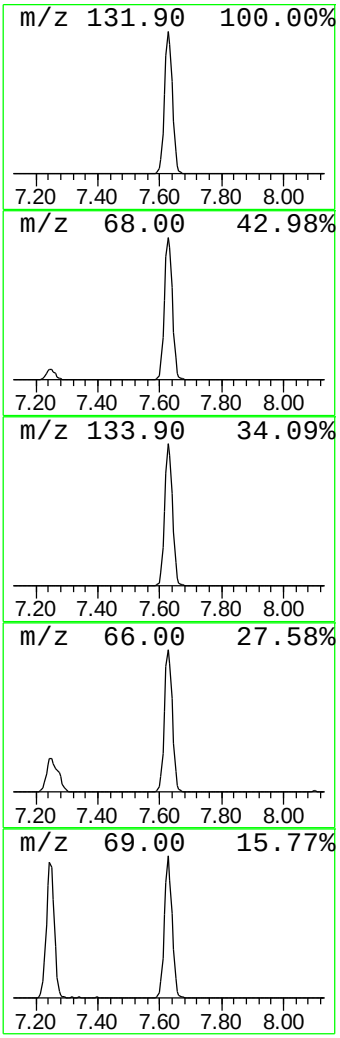
****

Peak Number 3 unknown7.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	121.40 ng	1750170	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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Instrument :
BNA_G
ClientSampleId :
DL-04A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101818.M
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TIC Library : C:\Database\NIST11.L
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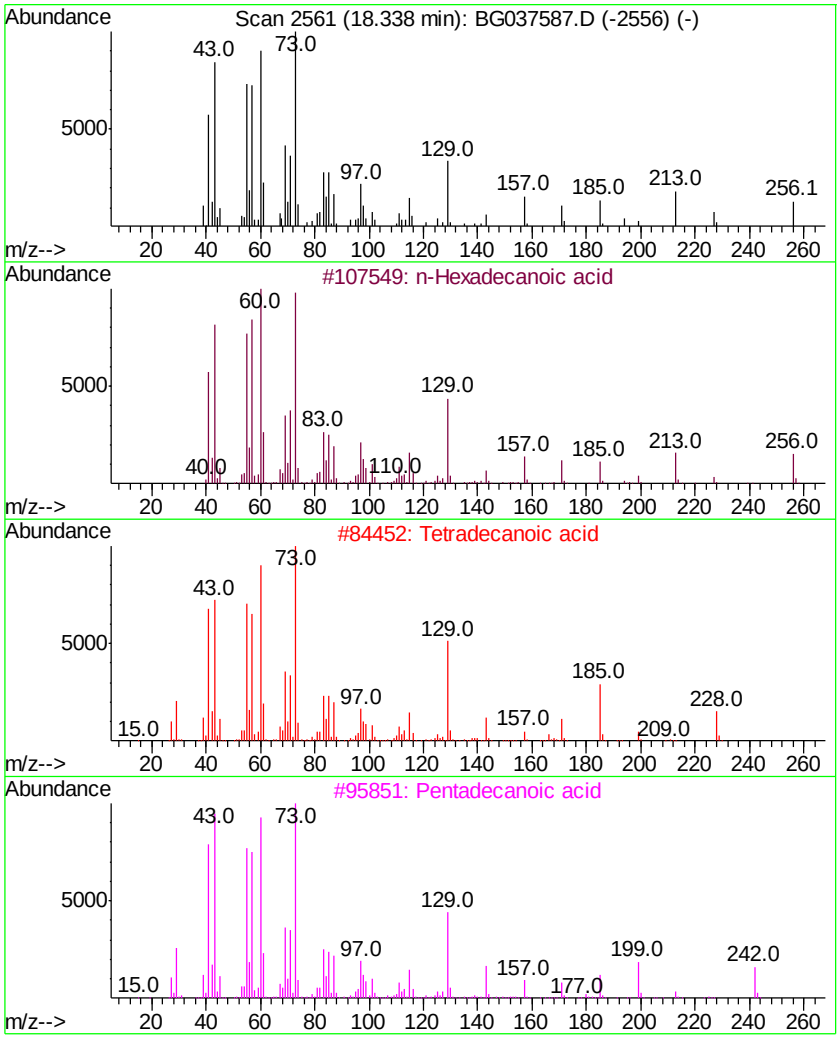
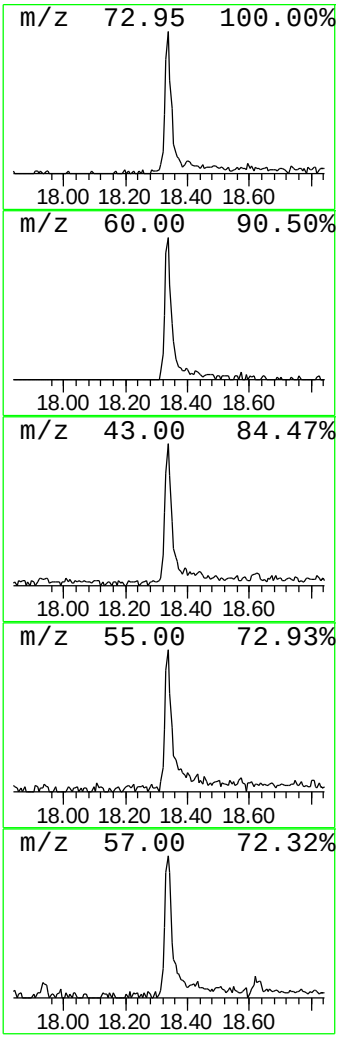
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	3.33 ng	149402	Phenanthrene-d10	17.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





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BNA_G
ClientSampleId :
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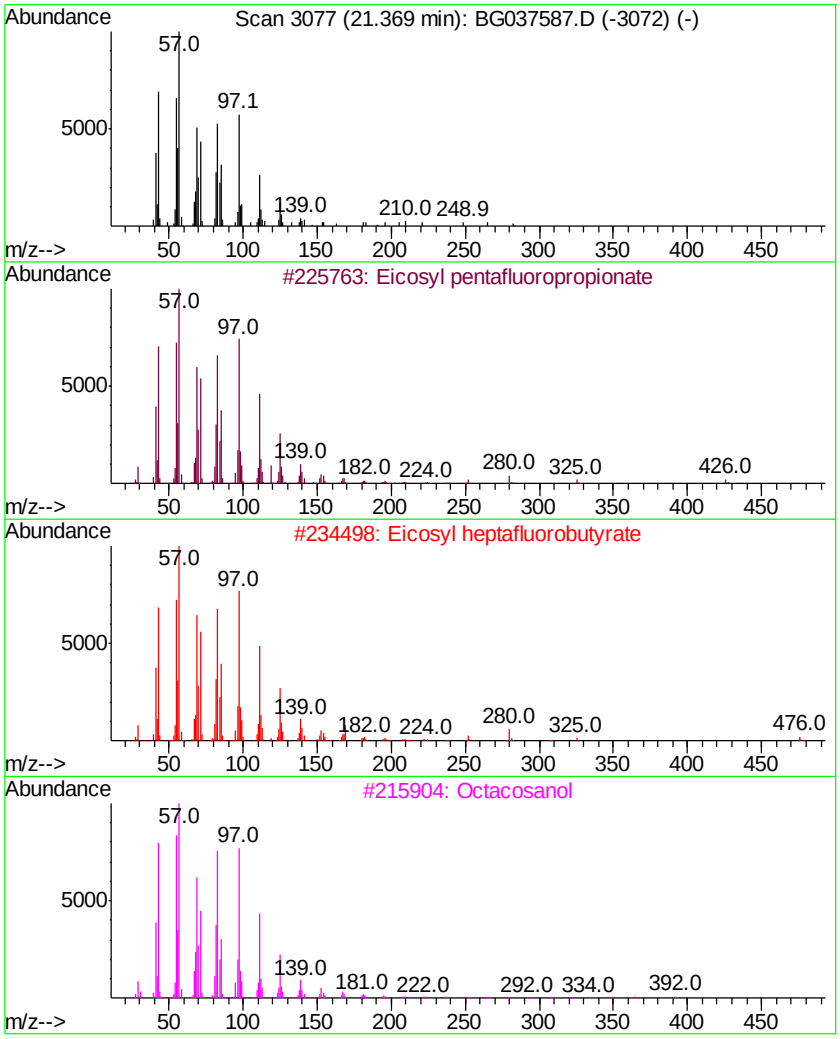
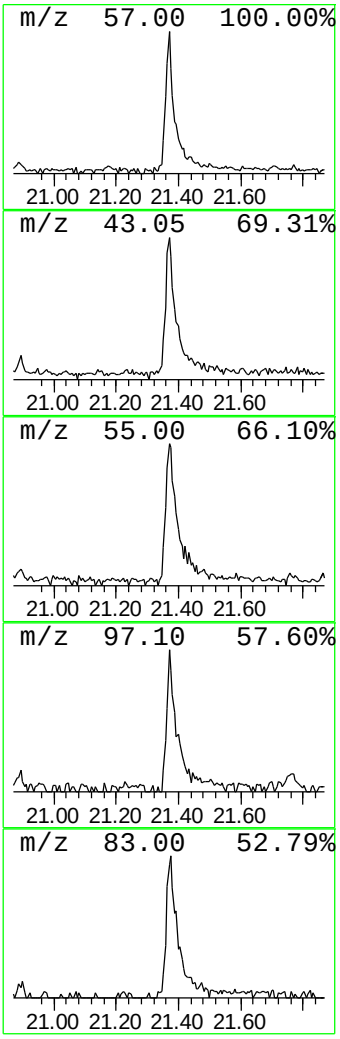
****

Peak Number 6 Eicosyl pentafluoropropionate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	3.45 ng	159180	Chrysene-d12	21.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
2	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3	Octacosanol	410	C28H58O	000557-61-9	90
4	17-Pentatriacontene	491	C35H70	006971-40-0	87
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
(S)-(+)-1,2-Propa...	3.77	5.0	ng	72304	1	8.10	288325	20.0
2-Pentanone, 4-hy...	5.18	6.0	ng	87082	1	8.10	288325	20.0
unknown7.63	7.63	121.4	ng	1750170	1	8.10	288325	20.0
n-Hexadecanoic acid	18.34	3.3	ng	149402	4	17.48	896093	20.0
Eicosyl pentafluo...	21.37	3.5	ng	159180	5	21.76	924097	20.0