LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG031318\
Data File : BG033116.D
Acq On : 13 Mar 2018 12:43
Operator : SJ/JU
Sample : J1873-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-9A-COMP

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:\HPCHEM1\BNA_G\METHODS\8270-BG022118.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	3.517	32	39	54	rVB2	30157	81743	3.38%	0.547%
2	5.820	426	431	437	rVB	20741	34652	1.43%	0.232%
3	6.325	510	517	530	rBV	711906	1223607	50.54%	8.190%
4	8.005	795	803	817	rBV	705076	1311175	54.16%	8.776%
5	8.423	865	874	888	rVB	693526	1272203	52.55%	8.515%
6	8.910	950	957	967	rVB	170503	303365	12.53%	2.030%
7	9.245	1006	1014	1026	rBV	501451	947946	39.15%	6.345%
8	10.109	1153	1161	1171	rBV	428541	796485	32.90%	5.331%
9	11.794	1439	1448	1457	rBV	246492	444408	18.36%	2.974%
10	14.150	1842	1849	1862	rVB	1078939	1722973	71.17%	11.532%
11	14.943	1978	1984	1989	rBV	61729	94093	3.89%	0.630%
12	15.354	2048	2054	2059	rVB	24183	30876	1.28%	0.207%
13	15.525	2076	2083	2091	rVB2	336591	558639	23.07%	3.739%
14	16.288	2209	2213	2218	rVB	28519	34854	1.44%	0.233%
15	16.993	2326	2333	2346	rBV	780206	1233071	50.93%	8.253%
16	17.146	2353	2359	2365	rBV	23373	36883	1.52%	0.247%
17	18.250	2540	2547	2554	rBV	423340	661138	27.31%	4.425%
18	19.043	2677	2682	2690	rBV	63794	99565	4.11%	0.666%
19	20.283	2888	2893	2895	rBV3	14421	24294	1.00%	0.163%
20	20.765	2970	2975	2985	rBV	1754704	2421093	100.00%	16.204%
21	22.122	3200	3206	3221	rBV	63428	177145	7.32%	1.186%
22	22.603	3280	3288	3297	rBV2	371613	714659	29.52%	4.783%
23	24.507	3605	3612	3618	rVB4	12637	29520	1.22%	0.198%
24	26.404	3920	3935	3952	rBV3	178338	686503	28.36%	4.595%

Sum of corrected areas: 14940890

LSC Report - Integrated Chromatogram

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Instrument :
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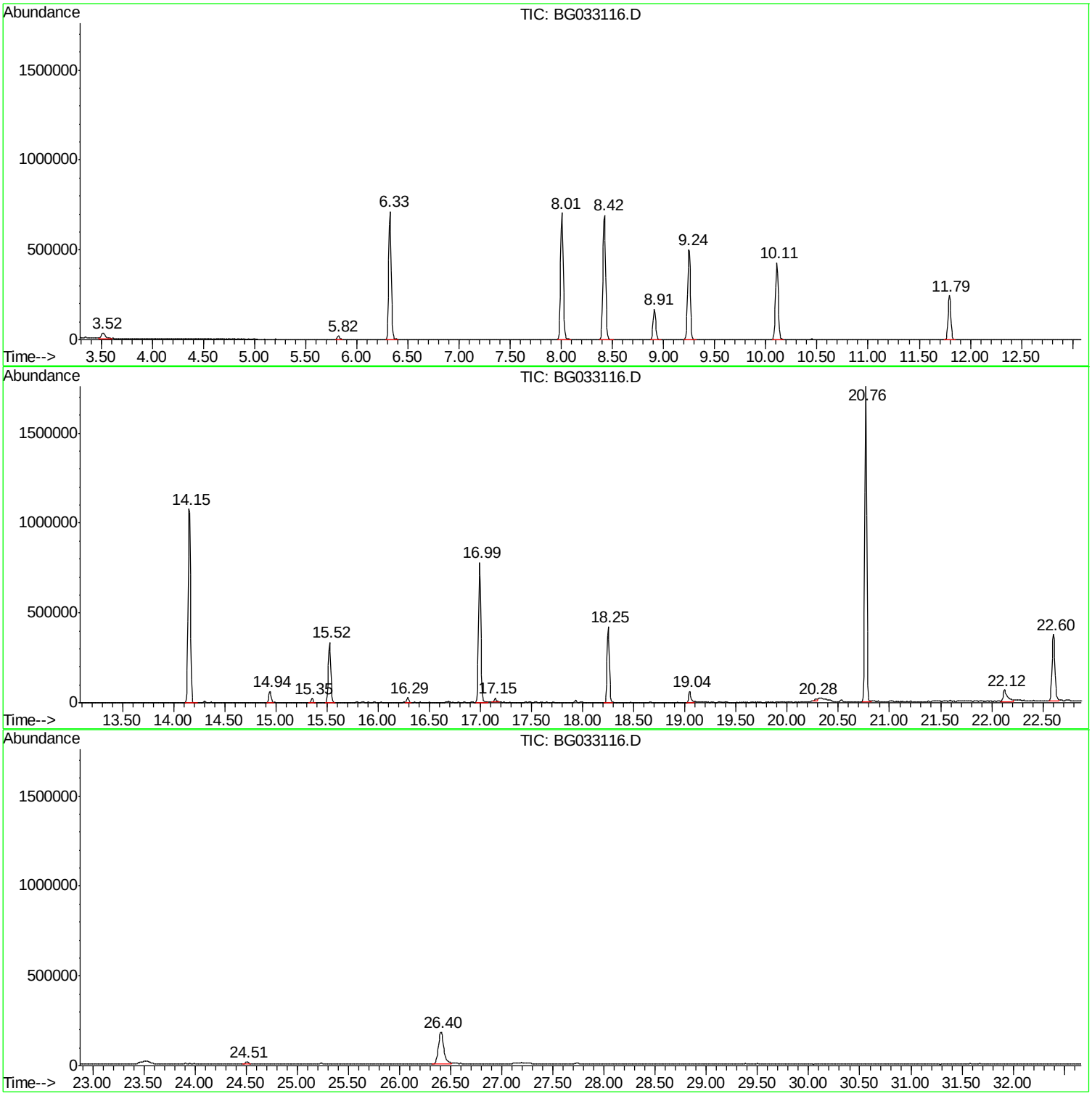
ClientSampleId :
TP-9A-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.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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Data File : BG033116.D
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Sample : J1873-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-9A-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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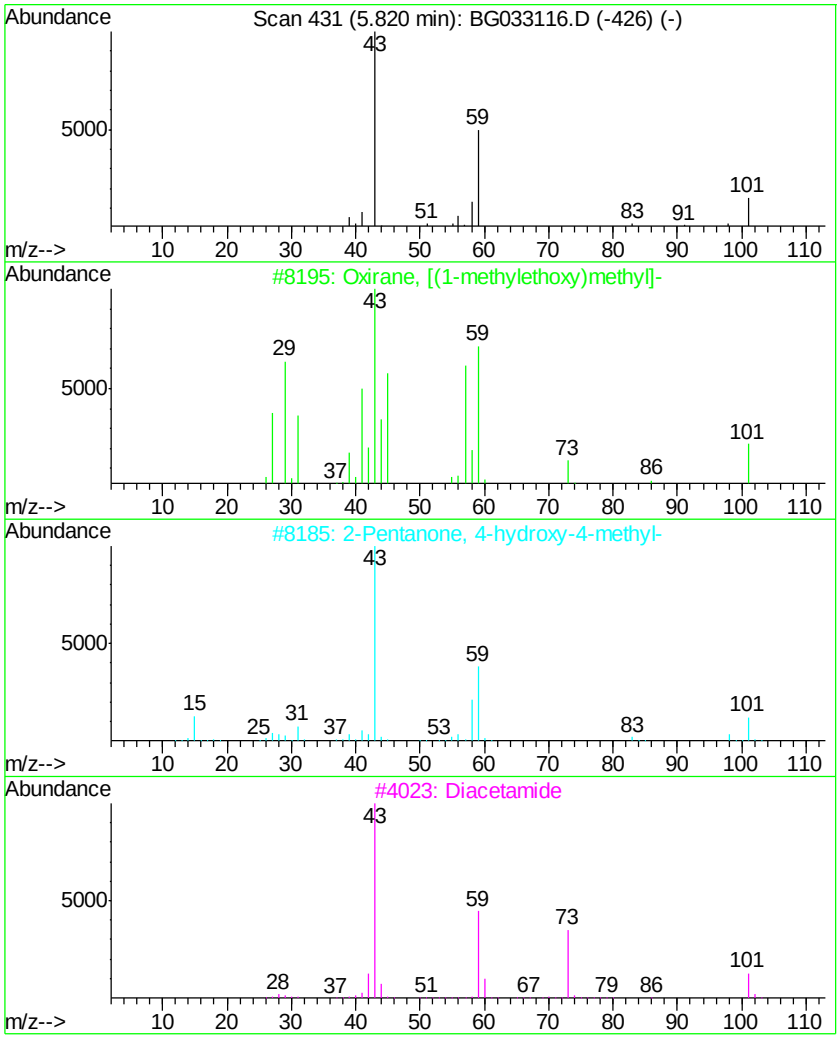
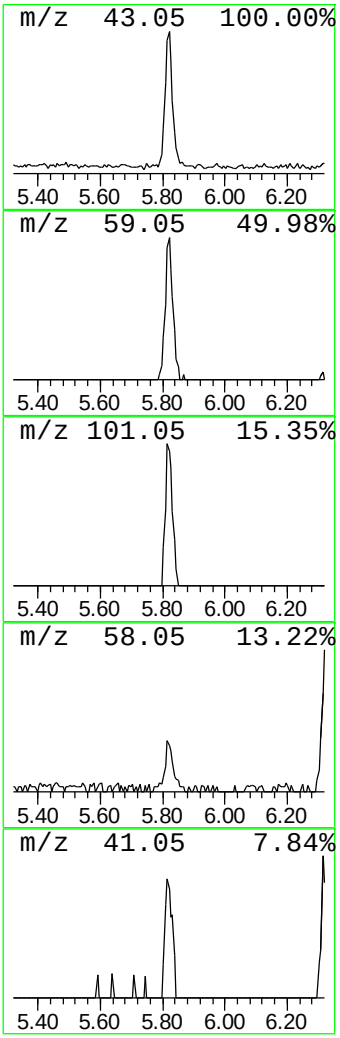
Peak Number 2 unknown5.82 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.82	2.28 ng	34652	1,4-Dichlorobenzene-d4	8.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	40
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
5	Butane	58	C4H10	000106-97-8	5





Library Search Compound Report

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Sample : J1873-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-9A-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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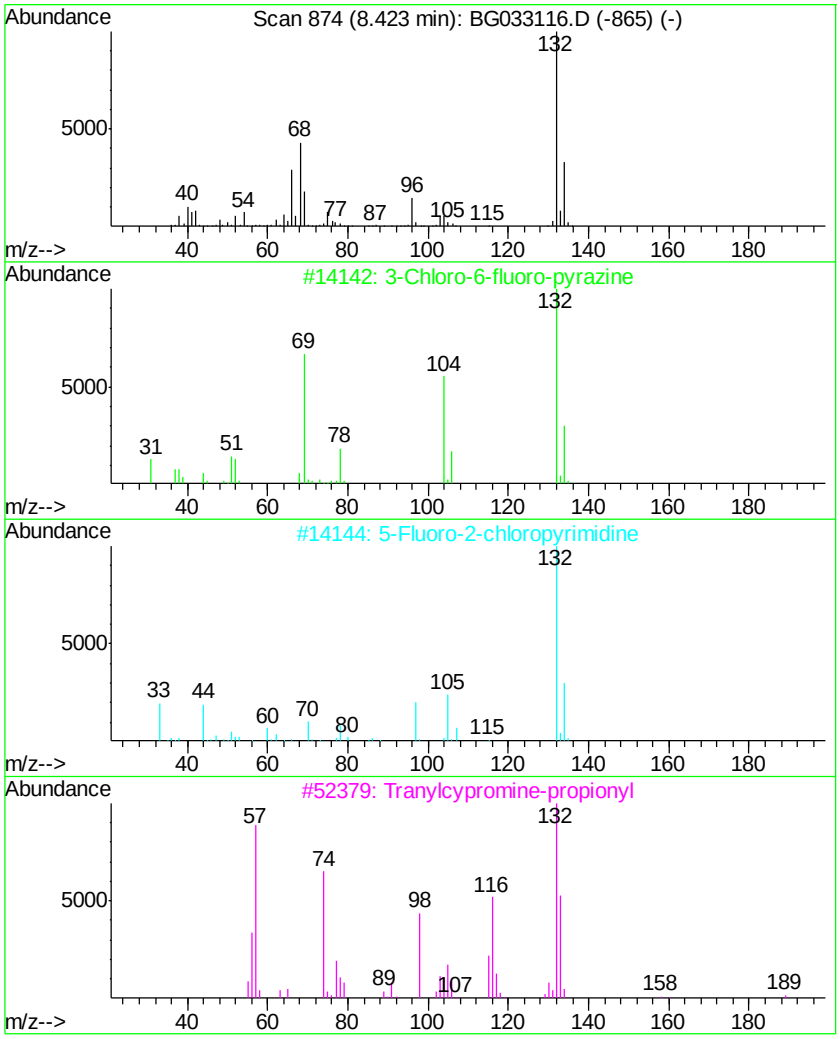
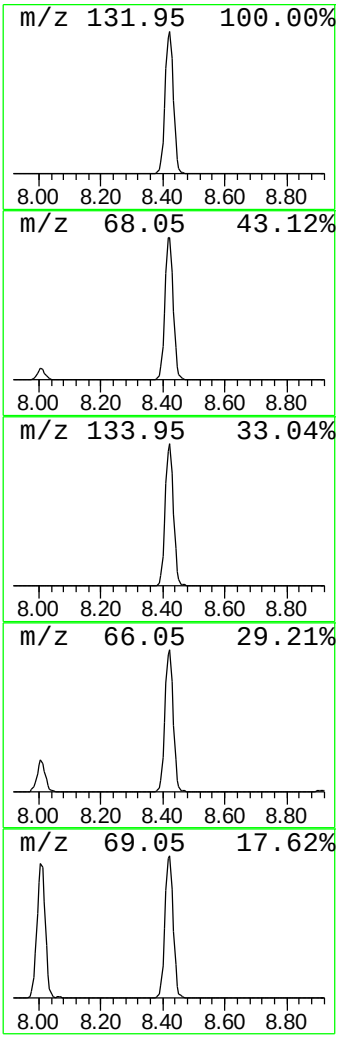
Peak Number 3 unknown8.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.42	83.87 ng	1272200	1,4-Dichlorobenzene-d4	8.91

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Data File : BG033116.D
Acq On : 13 Mar 2018 12:43
Operator : SJ/JU
Sample : J1873-06
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-9A-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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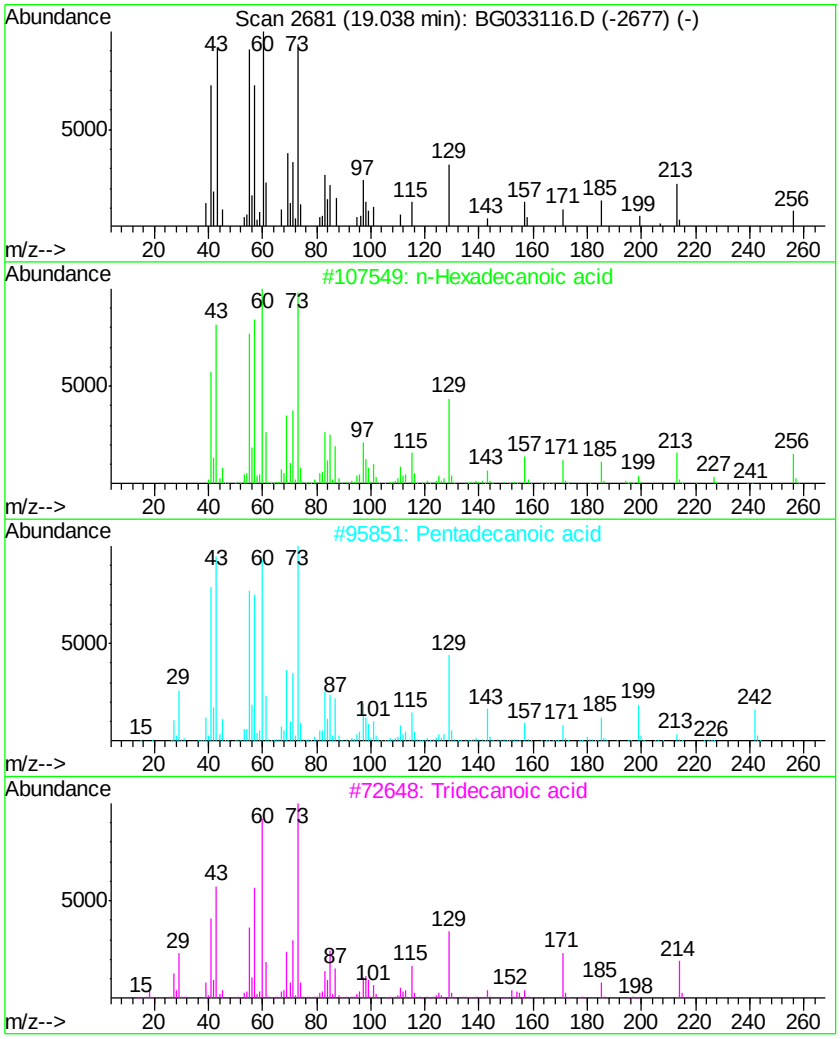
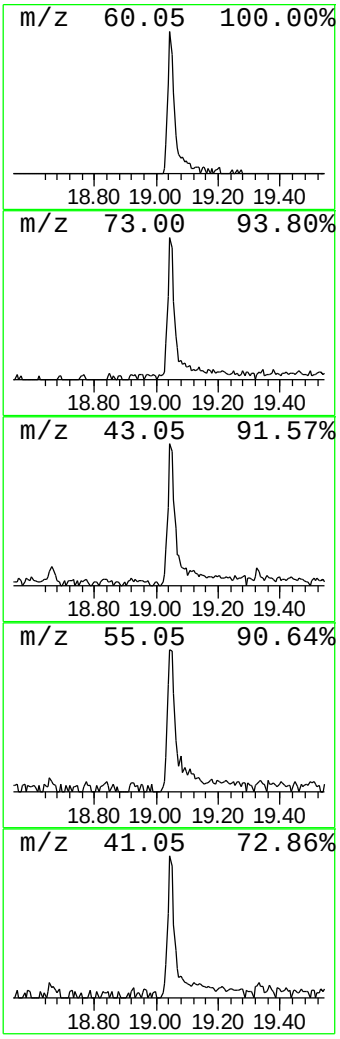
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.04	3.01 ng	99565	Phenanthrene-d10	18.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Instrument :
BNA_G
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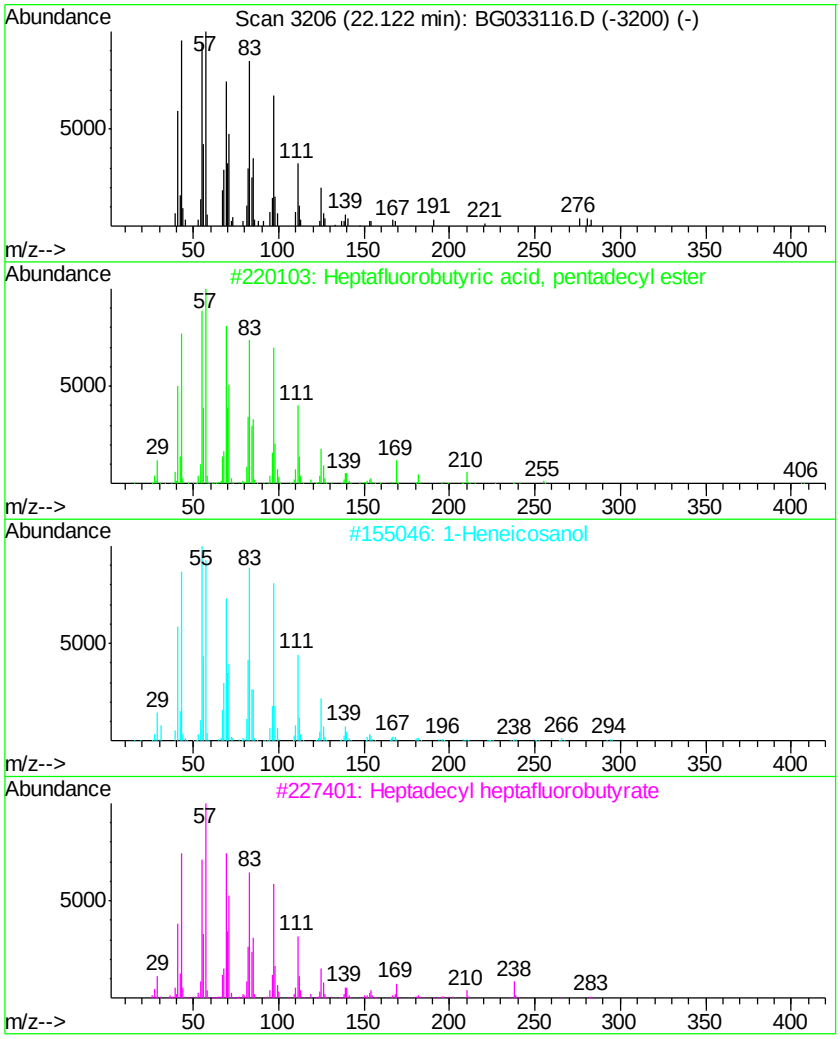
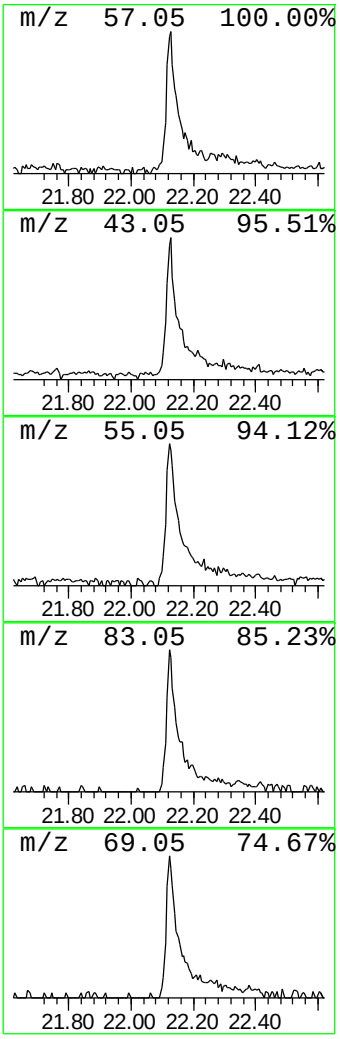
Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.12	4.96 ng	177145	Chrysene-d12	22.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Tentatively Identified Compound (LSC) summary

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Instrument :
BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022118.M
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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
unknown5.82	5.82	2.3	ng	34652	1	8.91	303365	20.0
unknown8.42	8.42	83.9	ng	1272200	1	8.91	303365	20.0
n-Hexadecanoic acid	19.04	3.0	ng	99565	4	18.25	661138	20.0
Heptafluorobutyri...	22.12	5.0	ng	177145	5	22.60	714659	20.0