LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102397.D
Acq On : 24 Jan 2018 18:45
Operator : SJ/JU
Sample : J1250-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AB-16(0-2)

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_F\METHODS\8270-BF012218.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	4.916	477	481	490	rVB	70395	95653	3.21%	0.376%
2	5.328	546	551	554	rBV	2813196	2740483	91.92%	10.768%
3	6.357	721	726	743	rBV	2526805	2981233	100.00%	11.714%
4	6.486	743	748	751	rBV	3177810	2835989	95.13%	11.143%
5	6.716	783	787	795	rBV	800339	672816	22.57%	2.644%
6	6.869	809	813	817	rBV	2380136	2136536	71.67%	8.395%
7	7.281	878	883	886	rBV	1784589	1784617	59.86%	7.012%
8	7.998	1001	1005	1018	rVB	991298	895627	30.04%	3.519%
9	8.557	1096	1100	1103	rBV	229426	198205	6.65%	0.779%
10	9.075	1183	1188	1191	rBV	3111476	2737537	91.83%	10.756%
11	9.469	1251	1255	1263	rBV	559925	469908	15.76%	1.846%
12	9.680	1288	1291	1294	rBV	55298	43299	1.45%	0.170%
13	9.751	1299	1303	1312	rVB	1073635	948954	31.83%	3.729%
14	10.180	1372	1376	1379	rVB2	59771	53088	1.78%	0.209%
15	10.463	1420	1424	1431	rBV	1134069	980804	32.90%	3.854%
16	10.539	1433	1437	1450	rVV	1549830	1572427	52.74%	6.178%
17	10.651	1453	1456	1461	rBV	56188	56787	1.90%	0.223%
18	11.098	1529	1532	1535	rBV	37718	31098	1.04%	0.122%
19	11.233	1552	1555	1563	rVB	927189	801120	26.87%	3.148%
20	12.821	1820	1825	1828	rBV	2091750	1913269	64.18%	7.518%
21	13.709	1973	1976	1983	rBV	162702	191893	6.44%	0.754%
22	13.868	2000	2003	2010	rVB	661298	644005	21.60%	2.530%
23	15.298	2241	2246	2252	rBV	517776	664968	22.31%	2.613%

Sum of corrected areas: 25450316

LSC Report - Integrated Chromatogram

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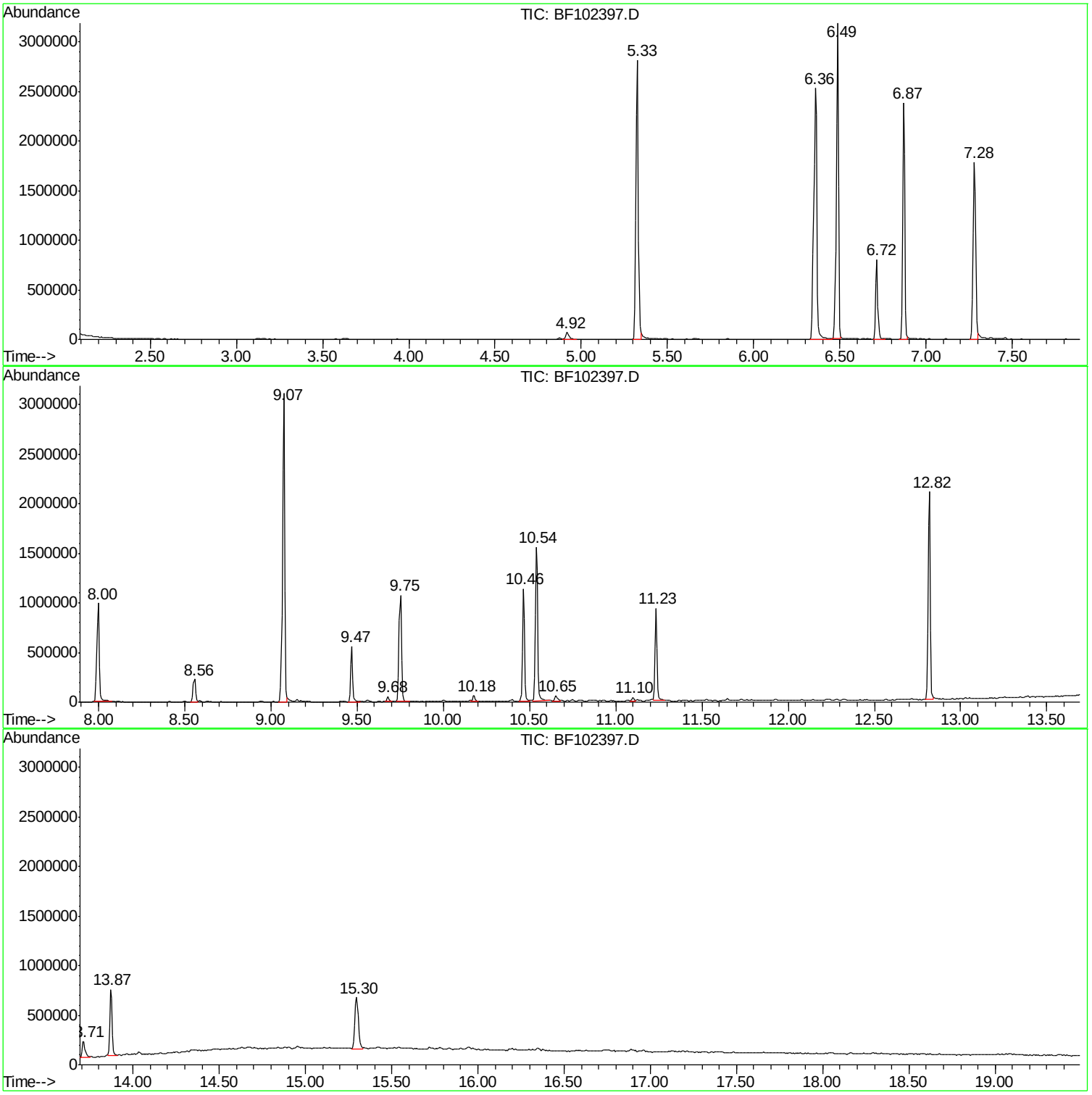
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AB-16(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102397.D
Acq On : 24 Jan 2018 18:45
Operator : SJ/JU
Sample : J1250-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AB-16(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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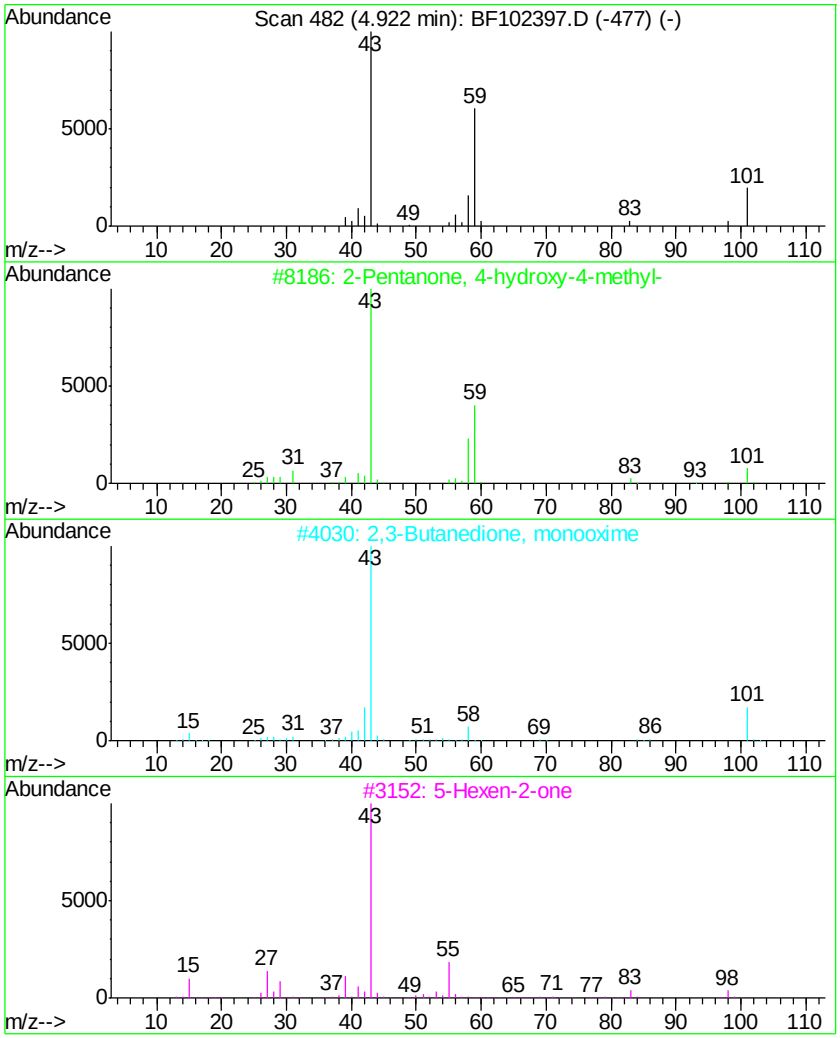
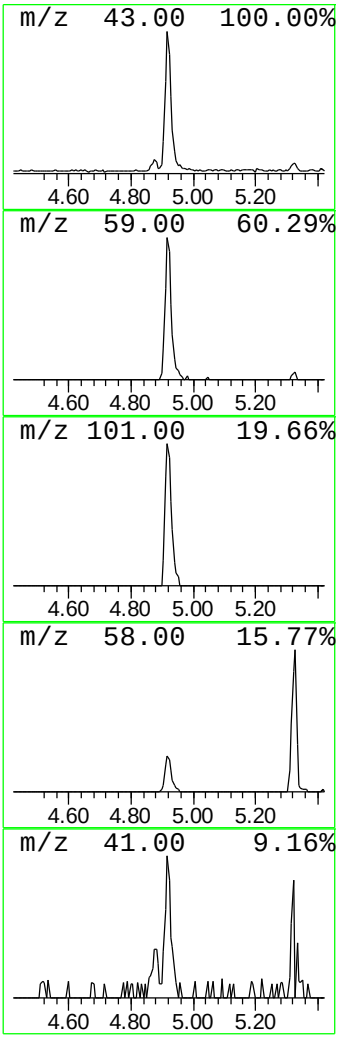
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.84 ng	95653	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	5-Hexen-2-one	98	C6H10O	000109-49-9	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propylamine	59	C3H9N	000107-10-8	9





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Sample : J1250-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AB-16(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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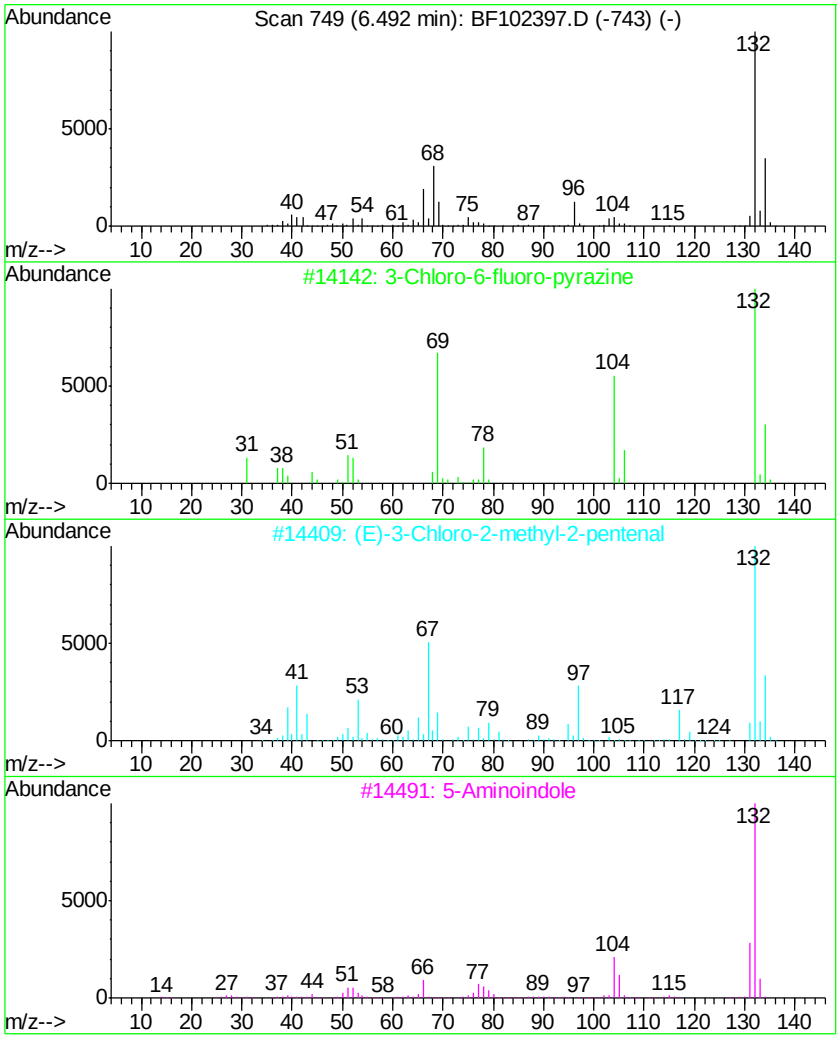
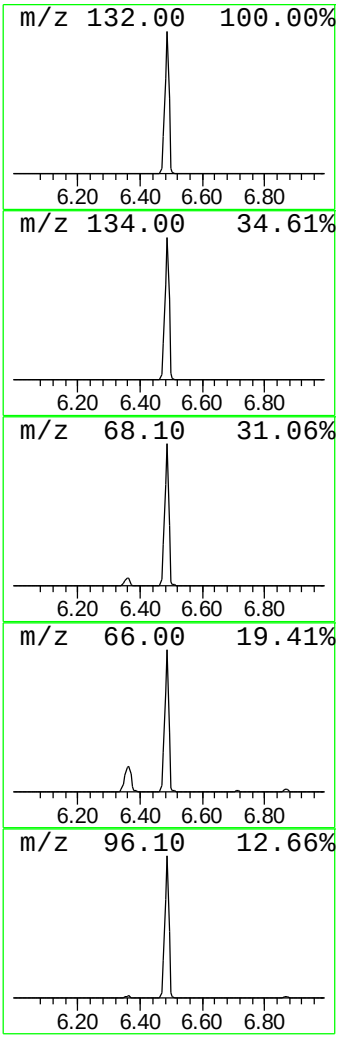
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	84.30 ng	2835990	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

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Data File : BF102397.D
Acq On : 24 Jan 2018 18:45
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Sample : J1250-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AB-16(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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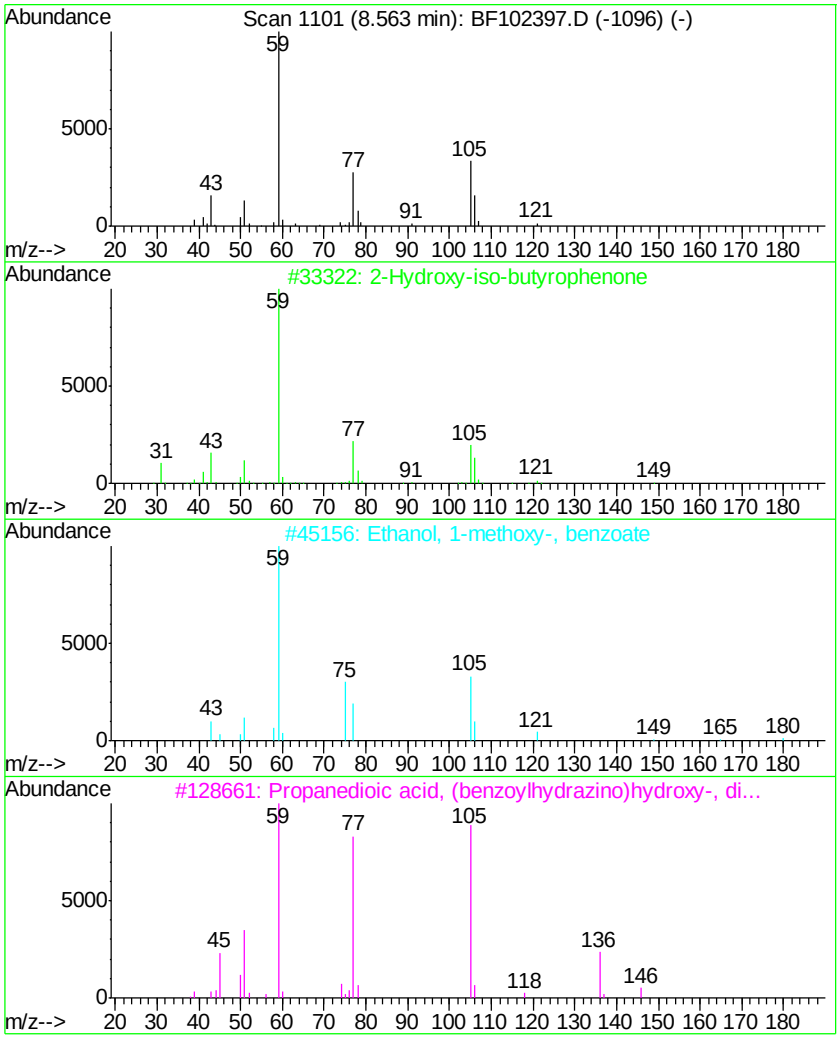
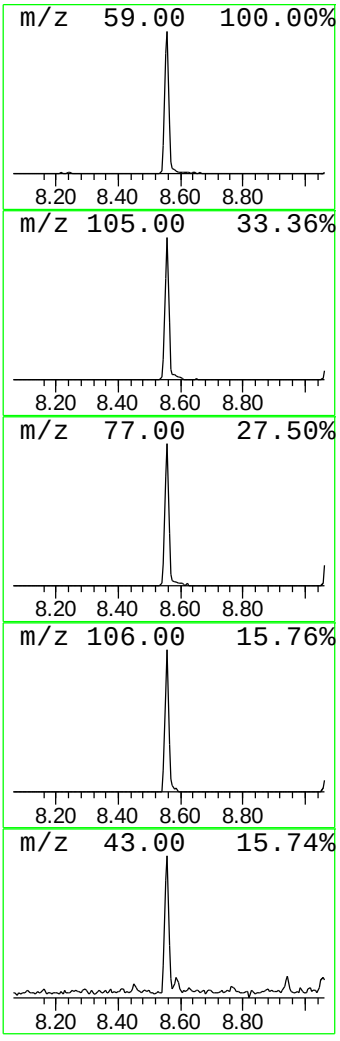
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	4.43 ng	198205	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	23
4	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	7





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Acq On : 24 Jan 2018 18:45
Operator : SJ/JU
Sample : J1250-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AB-16(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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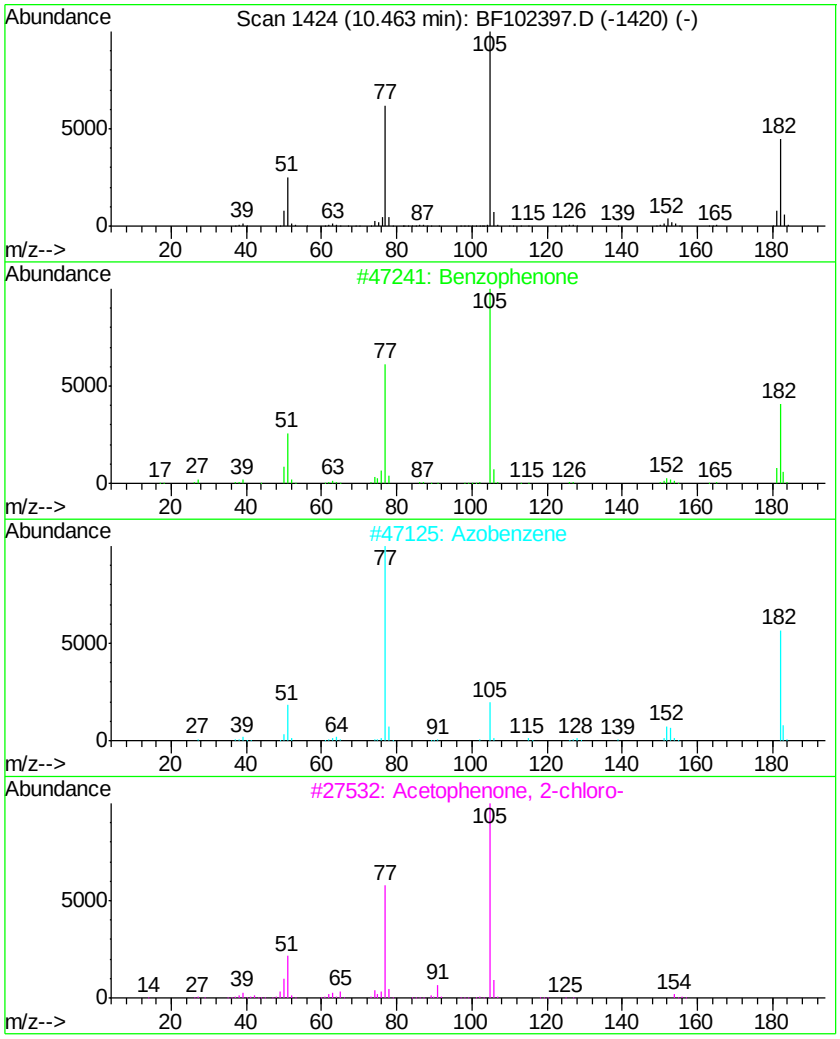
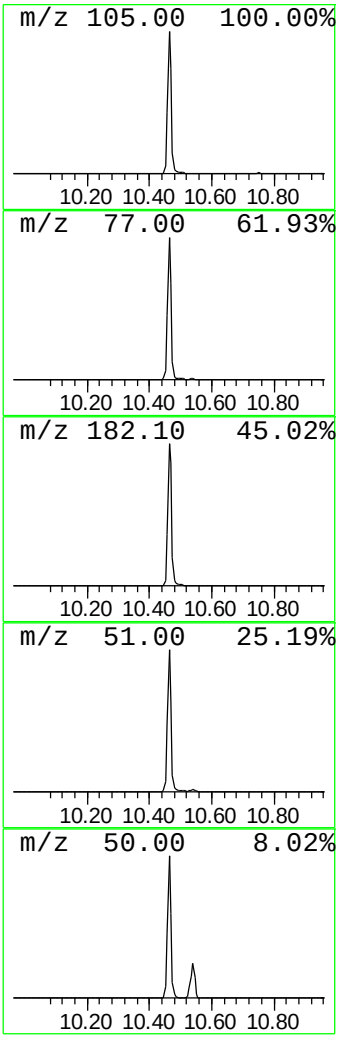
Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.46	20.67 ng	980804	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene	182	C12H10N2	000103-33-3	64
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47





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Operator : SJ/JU
Sample : J1250-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AB-16(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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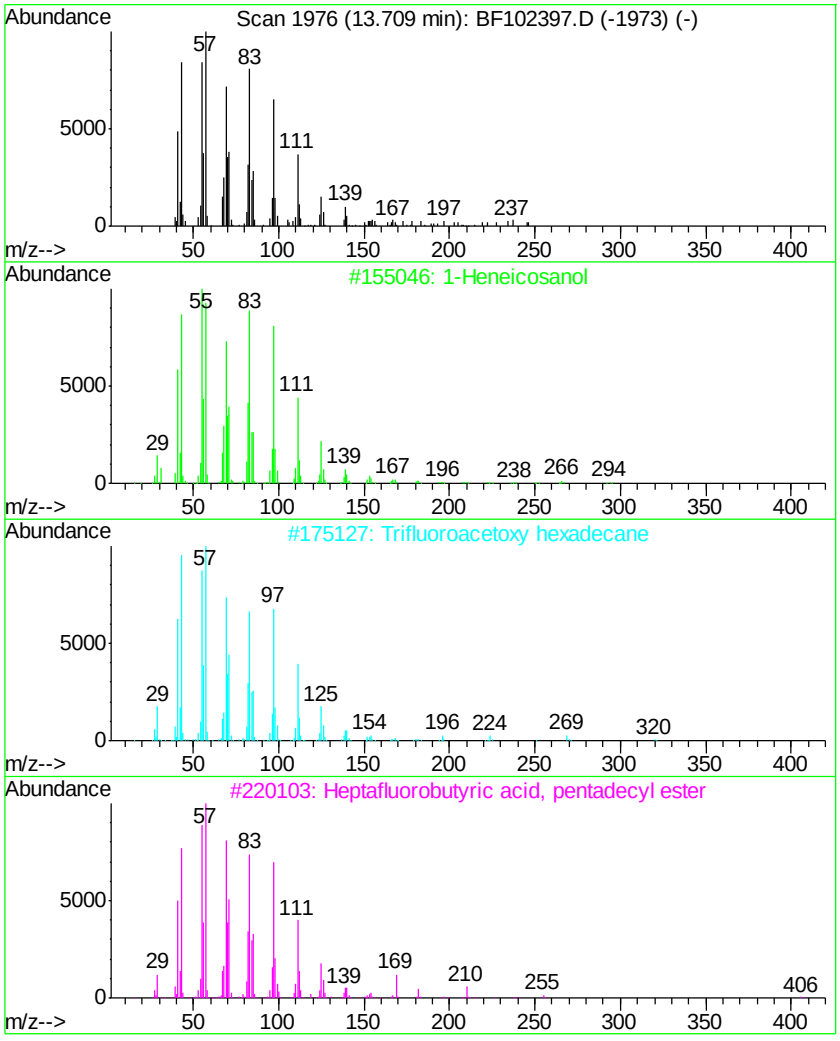
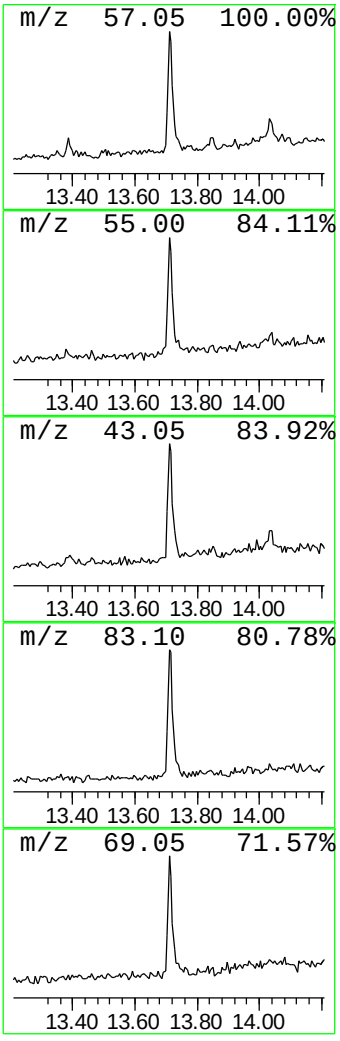
Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	5.96 ng	191893	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : AB-16(0-2)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	2.8	ng	95653	1	6.72	672816	20.0
unknown6.49	6.49	84.3	ng	2835990	1	6.72	672816	20.0
2-Hydroxy-iso-but...	8.56	4.4	ng	198205	2	8.00	895627	20.0
Benzophenone	10.46	20.7	ng	980804	3	9.75	948954	20.0
1-Heneicosanol	13.71	6.0	ng	191893	5	13.87	644005	20.0