LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089069.D
Acq On : 16 Jul 2016 22:13
Operator : UM/SJ
Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

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-BF063016.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	1.644	4	5	14	rVV	52343	126673	10.13%	1.032%
2	1.770	14	16	36	rVB	696051	1159202	92.69%	9.443%
3	4.799	279	281	286	rBB	84113	127600	10.20%	1.039%
4	5.267	319	322	324	rBV	765824	1051957	84.12%	8.569%
5	6.330	411	415	417	rBV	911440	1218851	97.46%	9.929%
6	6.445	422	425	427	rBB	880057	1145169	91.57%	9.329%
7	6.662	442	444	446	rBV	310861	326625	26.12%	2.661%
8	6.822	456	458	460	rVB	1046409	861278	68.87%	7.016%
9	7.233	491	494	496	rBV	752557	649058	51.90%	5.287%
10	7.953	555	557	559	rBV	585966	468393	37.45%	3.816%
11	9.028	649	651	654	rBV	941124	1250606	100.00%	10.188%
12	9.428	684	686	689	rBV	271188	217189	17.37%	1.769%
13	9.702	708	710	712	rBV	450307	407091	32.55%	3.316%
14	10.148	748	749	751	rVB	15284	14103	1.13%	0.115%
15	10.365	765	768	771	rBV	6494	12690	1.01%	0.103%
16	10.491	777	779	781	rBV	575413	495823	39.65%	4.039%
17	10.628	788	791	794	rVB	15067	26219	2.10%	0.214%
18	11.074	828	830	831	rBV	18137	18363	1.47%	0.150%
19	11.188	837	840	842	rBV	252245	358915	28.70%	2.924%
20	11.234	842	844	848	rVB2	20302	33074	2.64%	0.269%
21	11.794	891	893	896	rBV	12745	16341	1.31%	0.133%
22	12.388	943	945	947	rVB	67511	55708	4.45%	0.454%
23	12.617	962	965	967	rBV	68247	77569	6.20%	0.632%
24	12.662	967	969	972	rVB3	9649	13525	1.08%	0.110%
25	12.765	976	978	981	rVB	680652	854306	68.31%	6.959%
26	12.948	990	994	996	rBV	10567	15676	1.25%	0.128%
27	13.017	996	1000	1001	rBV3	13493	22824	1.83%	0.186%
28	13.142	1009	1011	1012	rBV2	11577	13169	1.05%	0.107%
29	13.474	1037	1040	1041	rBV2	7652	12832	1.03%	0.105%
30	13.565	1045	1048	1049	rBV3	10128	19864	1.59%	0.162%
31	13.680	1055	1058	1061	rBV	63724	89617	7.17%	0.730%
32	13.817	1067	1070	1071	rBV	286953	402109	32.15%	3.276%
33	13.920	1077	1079	1081	rVB2	14762	17164	1.37%	0.140%
34	14.000	1084	1086	1087	rBV	16383	16828	1.35%	0.137%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089069.D
Acq On : 16 Jul 2016 22:13
Operator : UM/SJ
Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.308	1111	1113	1118	rBV2	41049	77135	6.17%	0.628%
36	14.731	1148	1150	1152	rBV	67391	78992	6.32%	0.643%
37	14.902	1162	1165	1170	rBV2	66493	142415	11.39%	1.160%
38	15.188	1187	1190	1192	rBV	150838	196961	15.75%	1.604%
39	15.405	1207	1209	1213	rVB2	41768	69050	5.52%	0.562%
40	15.611	1225	1227	1230	rBV	66227	114759	9.18%	0.935%

Sum of corrected areas: 12275723

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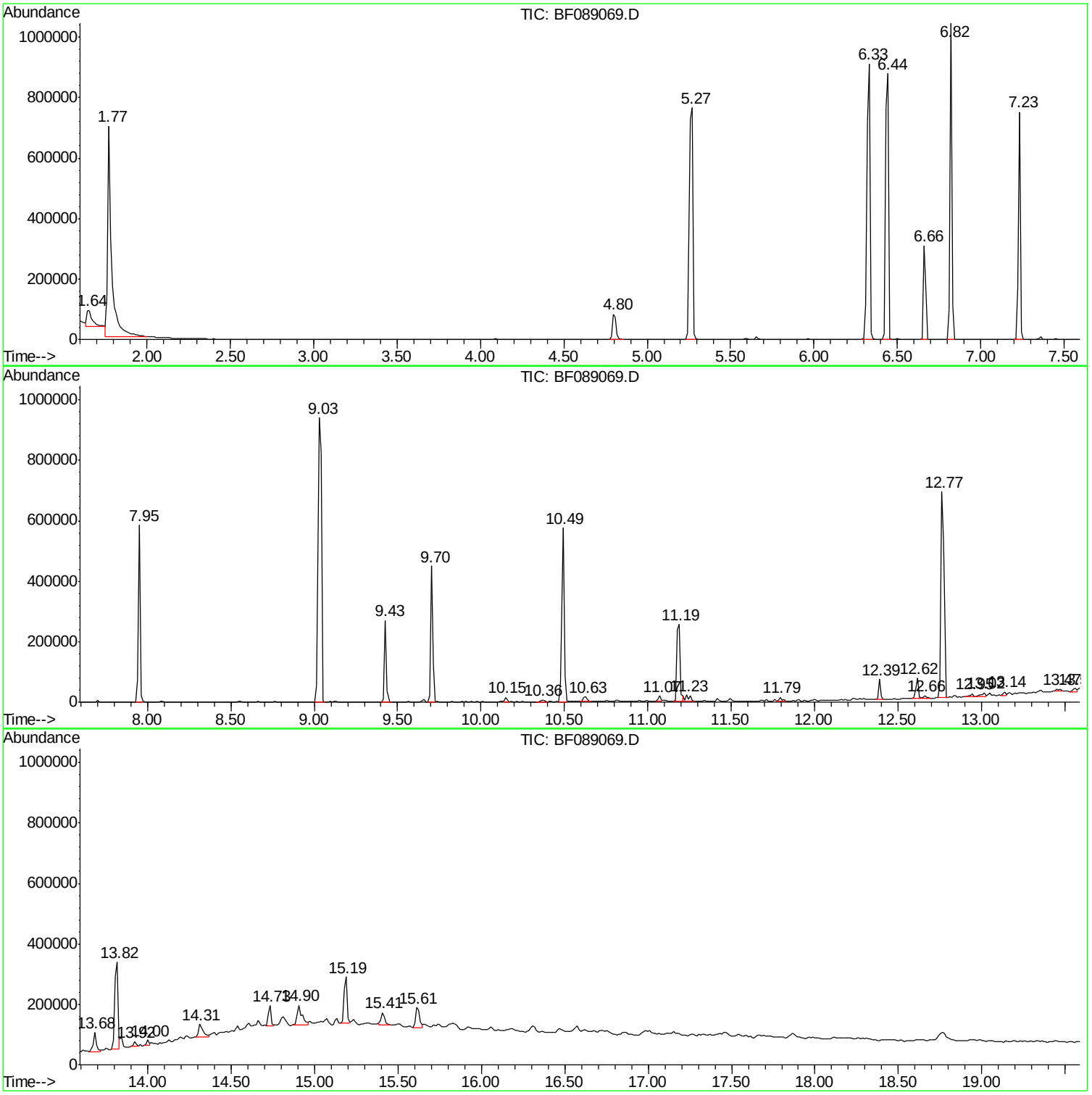
Acq On : 16 Jul 2016 22:13
Operator : UM/SJ
Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G9-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089069.D
Acq On : 16 Jul 2016 22:13
Operator : UM/SJ
Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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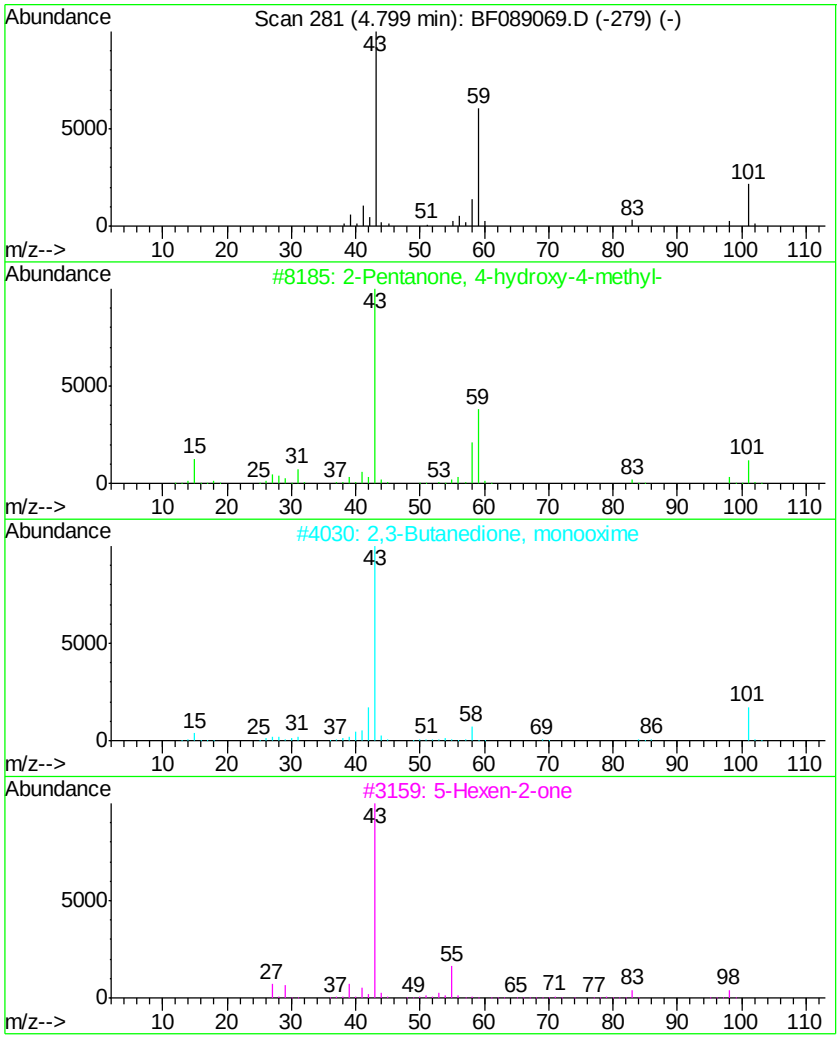
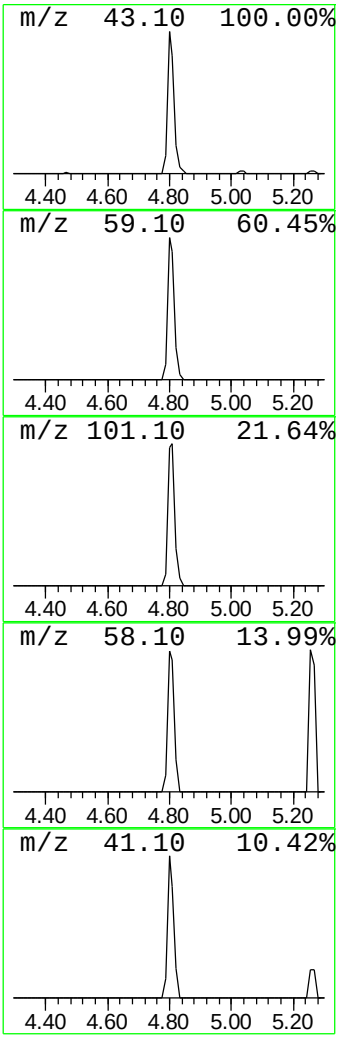
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	7.81 ng	127600	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089069.D
Acq On : 16 Jul 2016 22:13
Operator : UM/SJ
Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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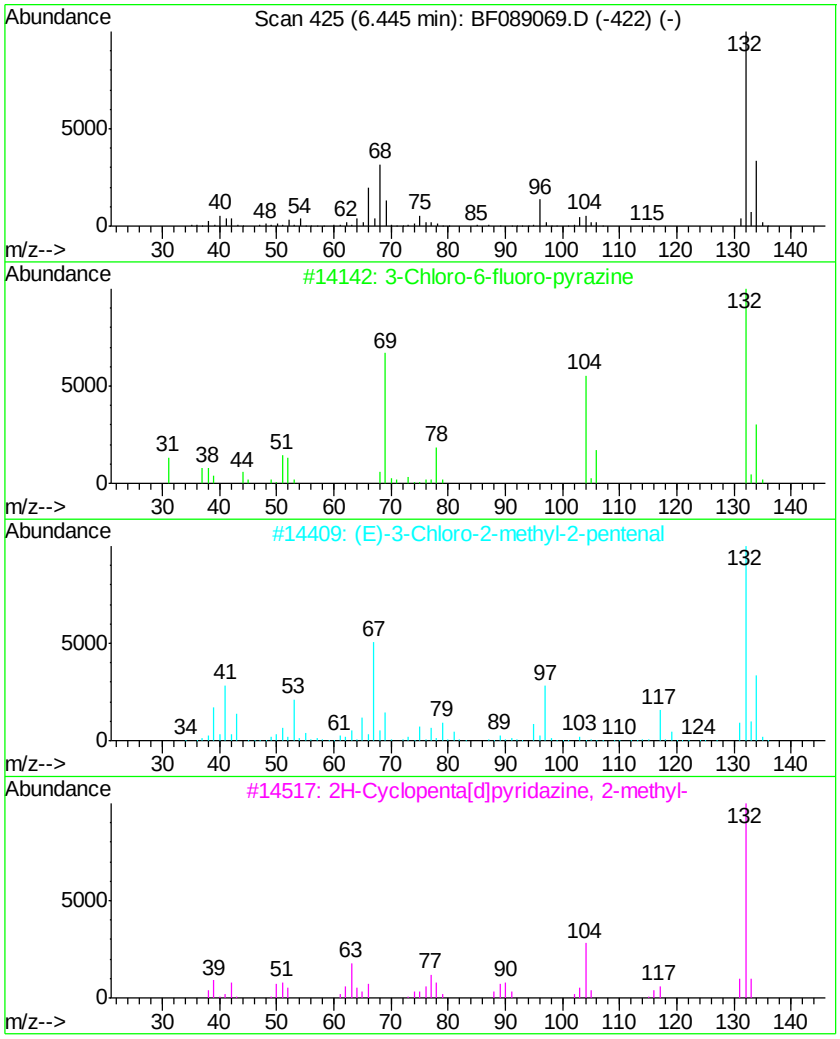
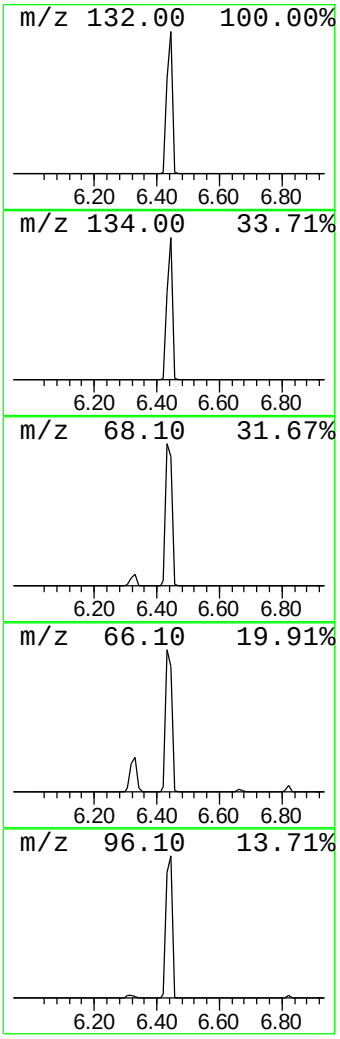
Peak Number 4 unknown6.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	70.12 ng	1145170	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089069.D
Acq On : 16 Jul 2016 22:13
Operator : UM/SJ
Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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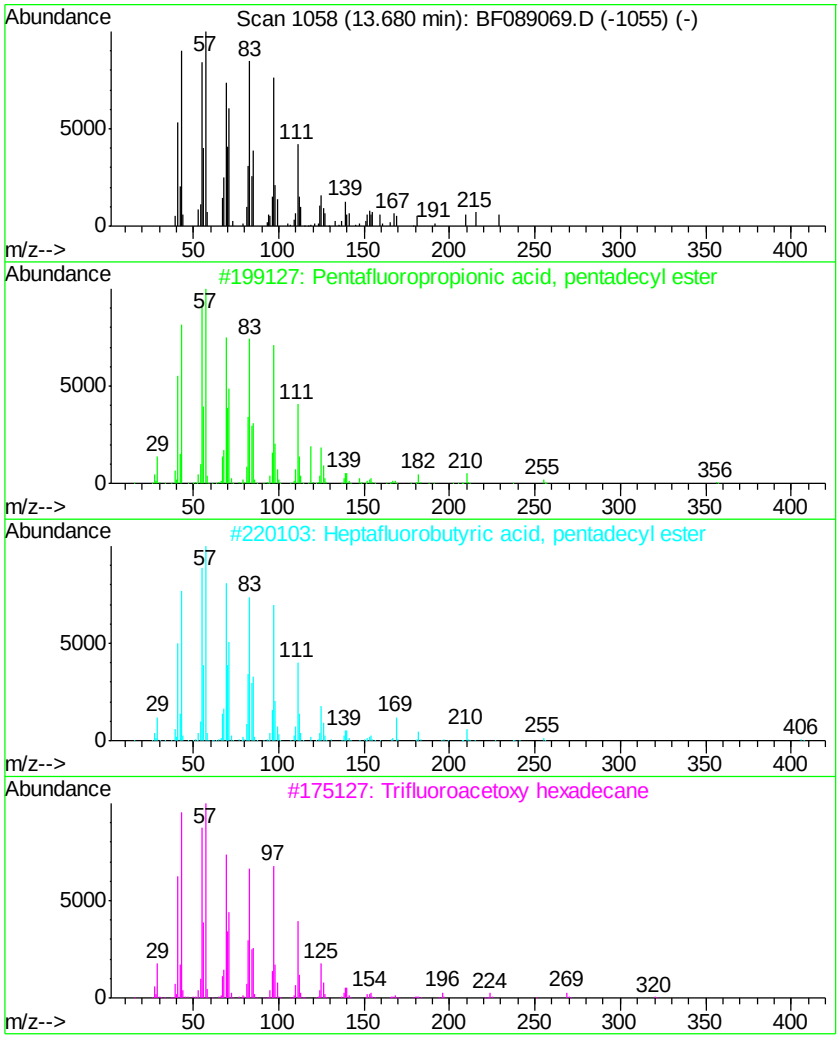
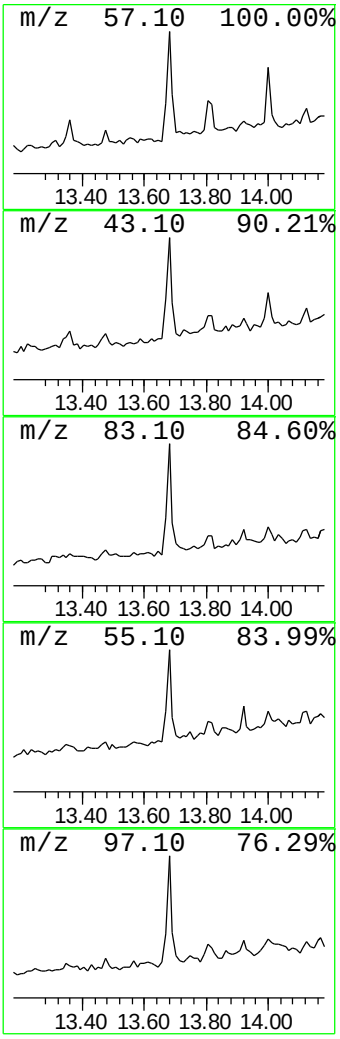
Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	4.46 ng	89617	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089069.D
Acq On : 16 Jul 2016 22:13
Operator : UM/SJ
Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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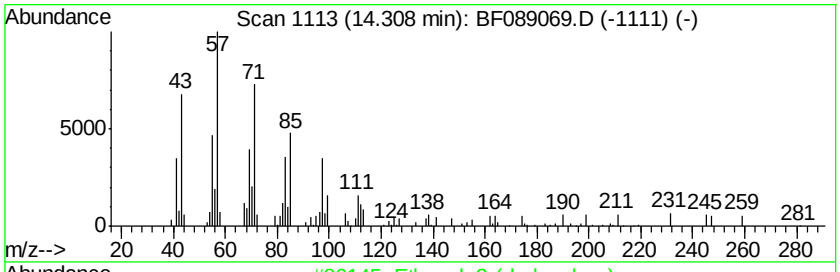
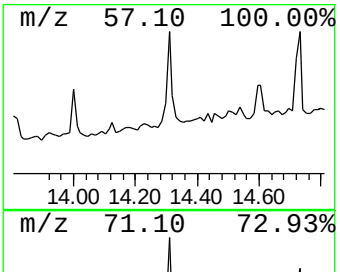
Peak Number 7 Ethanol, 2-(dodecyloxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	3.84 ng	77135	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	80
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	80
3	Nonadecane	268	C19H40	000629-92-5	52
4	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	50
5	Heneicosane	296	C21H44	000629-94-7	49





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071616\
Data File : BF089069.D
Acq On : 16 Jul 2016 22:13
Operator : UM/SJ
Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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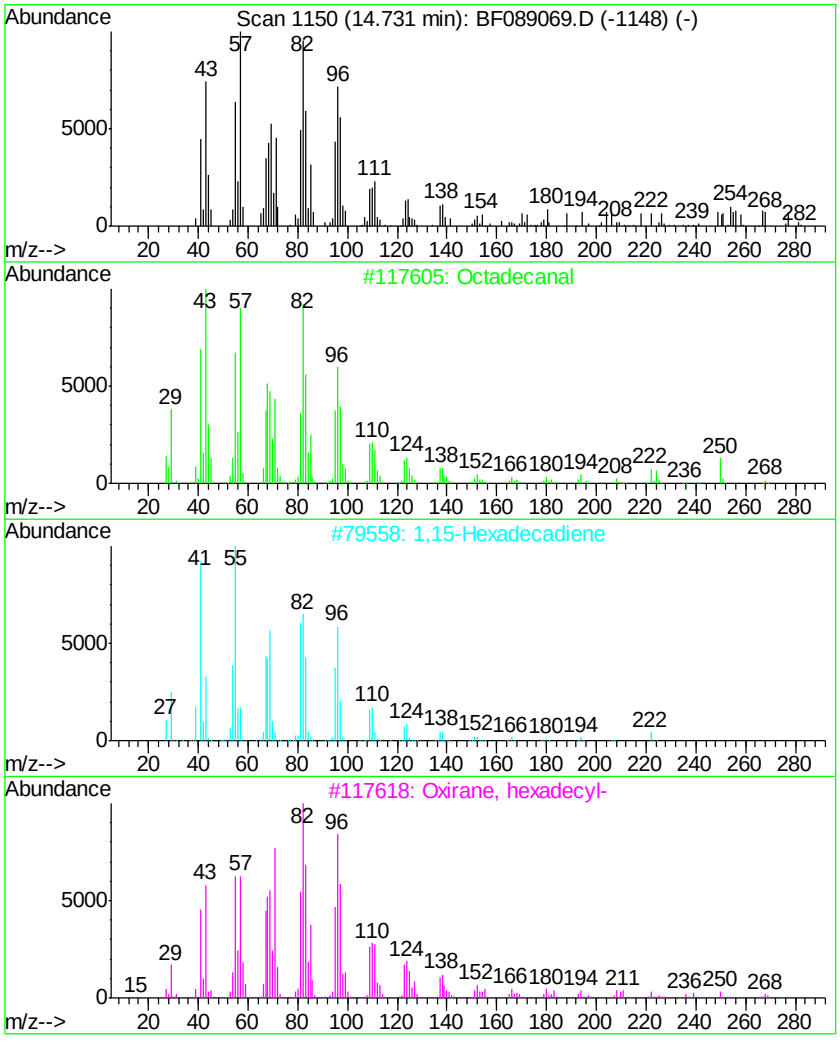
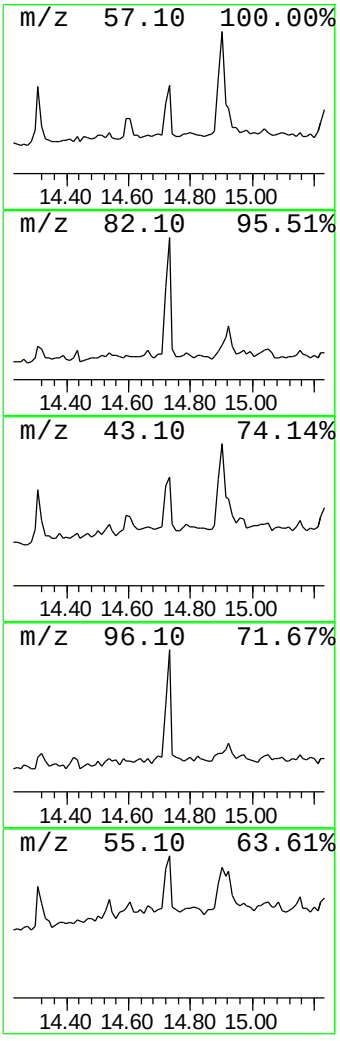
Peak Number 8 Octadecanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	8.02 ng	78992	Perylene-d12	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	90
2	1,15-Hexadecadiene	222	C16H30	021964-51-2	86
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	78
5	Hexadecanal	240	C16H32O	000629-80-1	74





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Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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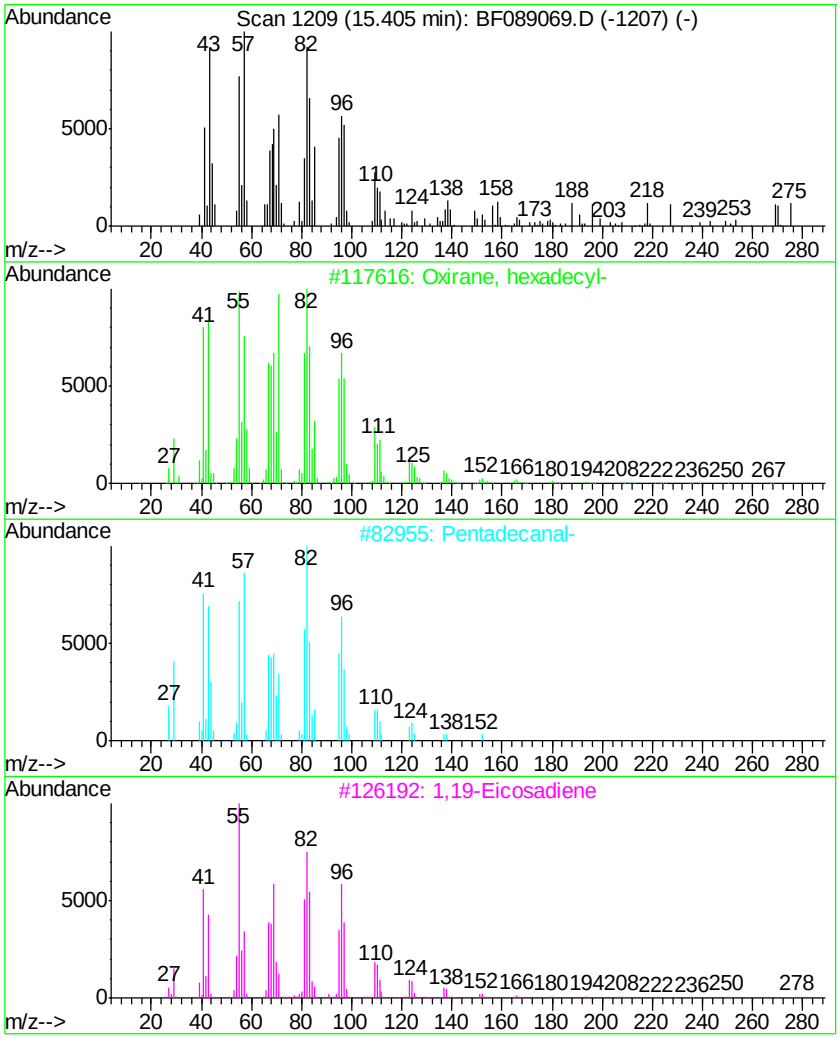
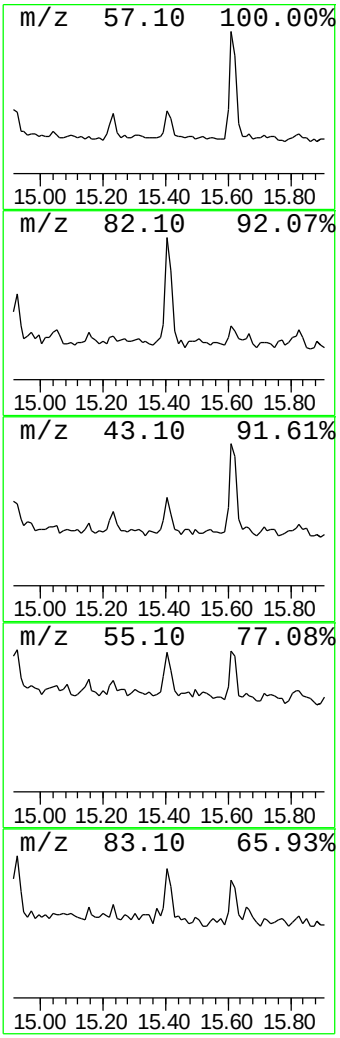
Peak Number 10 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.41	7.01 ng	69050	Perylene-d12	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	81
2	Pentadecanal-	226	C15H30O	002765-11-9	70
3	1,19-Eicosadiene	278	C20H38	014811-95-1	64
4	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	64
5	Octadecanal	268	C18H36O	000638-66-4	58





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Sample : H4018-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

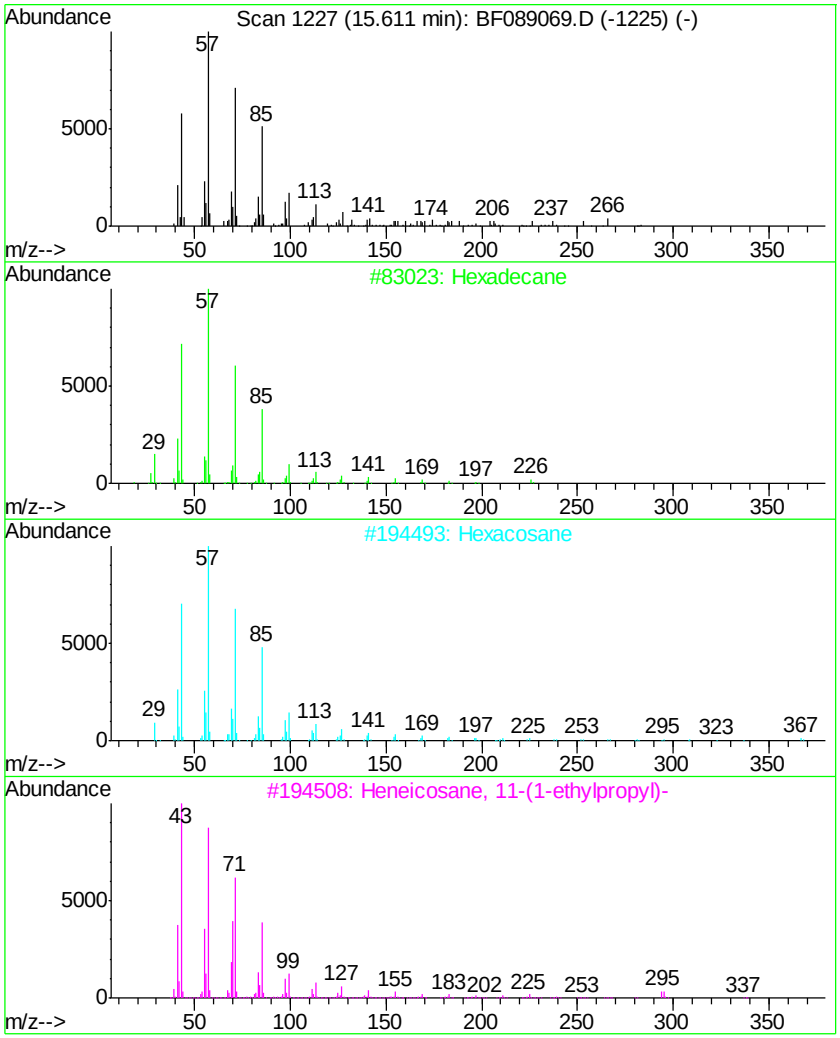
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

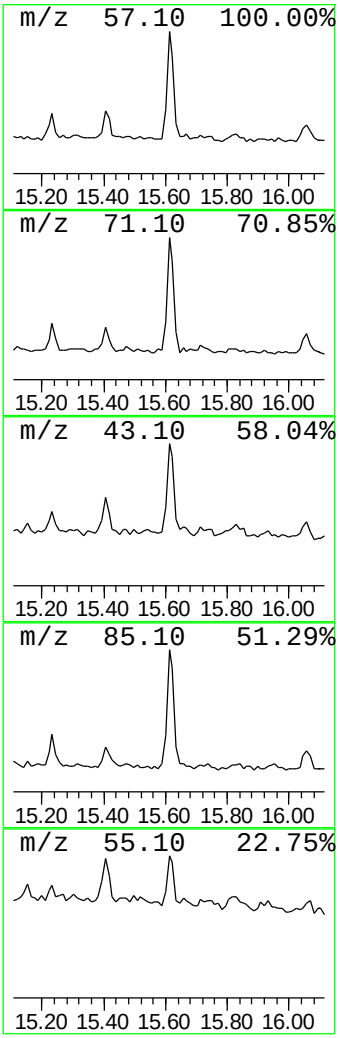
****

Peak Number 11 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	11.65 ng	114759	Perylene-d12	15.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071616\
Data File : BF089069.D
Acq On : 16 Jul 2016 22:13
Operator : UM/SJ
Sample : H4018-10
Misc :
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Instrument : BNA_F
ClientSampleId : G9-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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...	4.80	7.8	ng	127600	1	6.66	326625	20.0
unknown6.44	6.44	70.1	ng	1145170	1	6.66	326625	20.0
Pentafluoropropio...	13.68	4.5	ng	89617	5	13.82	402109	20.0
Ethanol, 2-(dodec...	14.31	3.8	ng	77135	5	13.82	402109	20.0
Octadecanal	14.73	8.0	ng	78992	6	15.19	196961	20.0
Oxirane, hexadecyl-	15.41	7.0	ng	69050	6	15.19	196961	20.0
Hexadecane	15.61	11.7	ng	114759	6	15.19	196961	20.0