LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

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-BF090115.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	4.399	243	246	258	rVB	464429	825155	52.12%	5.453%
2	4.901	288	290	293	rBV	1205330	1377298	87.00%	9.102%
3	6.022	385	388	391	rBV	1110286	1407198	88.89%	9.300%
4	6.124	395	397	399	rBV	1662196	1509116	95.33%	9.974%
5	6.353	415	417	420	rVB	390074	339337	21.44%	2.243%
6	6.513	428	431	433	rBV	1311131	1159091	73.22%	7.660%
7	6.936	465	468	470	rBV	1006432	1022289	64.58%	6.756%
8	7.085	478	481	483	rBV	17243	19150	1.21%	0.127%
9	7.645	528	530	532	rBV	504592	424406	26.81%	2.805%
10	8.730	622	625	627	rBV	1732578	1583038	100.00%	10.462%
11	9.130	658	660	663	rBV	273438	224694	14.19%	1.485%
12	9.382	680	682	685	rVB	424800	403888	25.51%	2.669%
13	10.171	748	751	753	rBV	833605	854428	53.97%	5.647%
14	10.319	762	764	769	rBV	20618	22780	1.44%	0.151%
15	10.845	808	810	813	rBV	357997	388880	24.57%	2.570%
16	11.119	832	834	838	rBV	102687	128525	8.12%	0.849%
17	11.188	838	840	843	rVB	20347	20800	1.31%	0.137%
18	11.428	858	861	864	rBV	43401	61787	3.90%	0.408%
19	11.668	881	882	887	rVB	41364	46272	2.92%	0.306%
20	11.931	903	905	908	rBV	74075	106566	6.73%	0.704%
21	11.976	908	909	911	rVB	63183	47851	3.02%	0.316%
22	12.342	938	941	946	rBV2	21595	32291	2.04%	0.213%
23	12.434	946	949	951	rBV	1253670	1089381	68.82%	7.200%
24	12.697	970	972	975	rVB	91492	82762	5.23%	0.547%
25	13.039	999	1002	1009	rVB	13937	21924	1.38%	0.145%
26	13.154	1009	1012	1013	rBV	15425	16781	1.06%	0.111%
27	13.359	1028	1030	1036	rBV	111250	173635	10.97%	1.148%
28	13.451	1036	1038	1041	rBV	238635	274520	17.34%	1.814%
29	13.794	1066	1068	1071	rBV	15933	17198	1.09%	0.114%
30	13.988	1082	1085	1088	rBV	74863	125054	7.90%	0.826%
31	14.400	1118	1121	1123	rBV	40367	51550	3.26%	0.341%
32	14.560	1133	1135	1139	rBV2	59698	169482	10.71%	1.120%
33	14.617	1139	1140	1142	rVB	24740	19899	1.26%	0.132%
34	14.765	1150	1153	1156	rVB	243746	238505	15.07%	1.576%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

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-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.902	1161	1165	1168	rVV3	6071	16758	1.06%	0.111%
36	14.982	1169	1172	1175	rBV	72763	84383	5.33%	0.558%
37	15.154	1185	1187	1189	rBV	46215	51570	3.26%	0.341%
38	15.200	1189	1191	1193	rVV	40716	73702	4.66%	0.487%
39	15.234	1193	1194	1197	rVB	34792	47999	3.03%	0.317%
40	15.325	1200	1202	1206	rVB4	14259	29030	1.83%	0.192%
41	15.405	1206	1209	1212	rBV4	7378	20711	1.31%	0.137%
42	15.623	1225	1228	1234	rVB5	10414	25154	1.59%	0.166%
43	15.725	1234	1237	1240	rBV	38404	59733	3.77%	0.395%
44	15.943	1253	1256	1258	rBV	12929	24634	1.56%	0.163%
45	16.011	1260	1262	1264	rVV3	11351	23624	1.49%	0.156%
46	16.068	1264	1267	1272	rVB2	32560	73165	4.62%	0.484%
47	16.274	1281	1285	1289	rBV5	10983	37826	2.39%	0.250%
48	16.354	1289	1292	1297	rVB5	14141	39705	2.51%	0.262%
49	16.480	1299	1303	1309	rBV7	11913	46341	2.93%	0.306%
50	16.743	1322	1326	1329	rBV5	7434	23494	1.48%	0.155%
51	16.960	1343	1345	1351	rVB4	9657	27246	1.72%	0.180%
52	17.188	1363	1365	1371	rVB4	12184	33501	2.12%	0.221%
53	17.588	1394	1400	1402	rBV5	7216	27749	1.75%	0.183%
54	17.691	1405	1409	1415	rVB4	26472	79242	5.01%	0.524%

Sum of corrected areas: 15131098

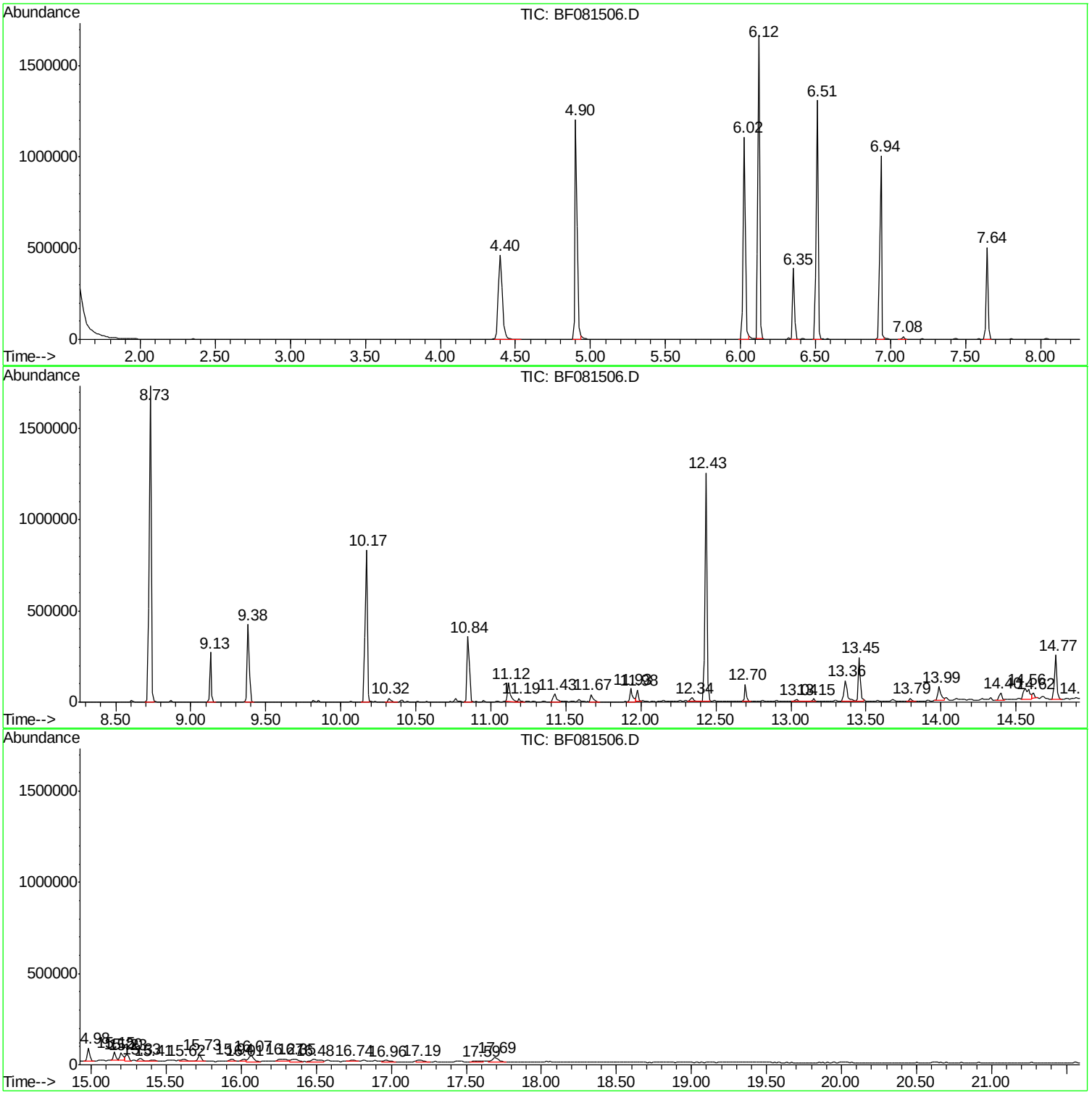
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

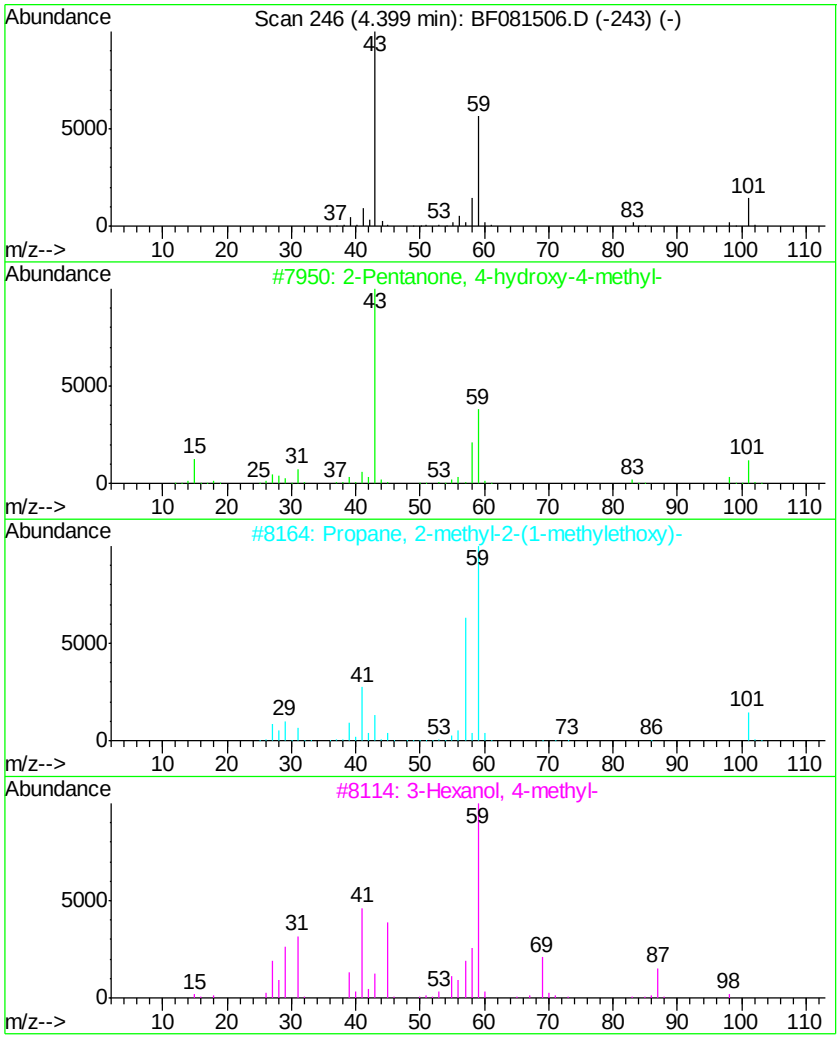
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

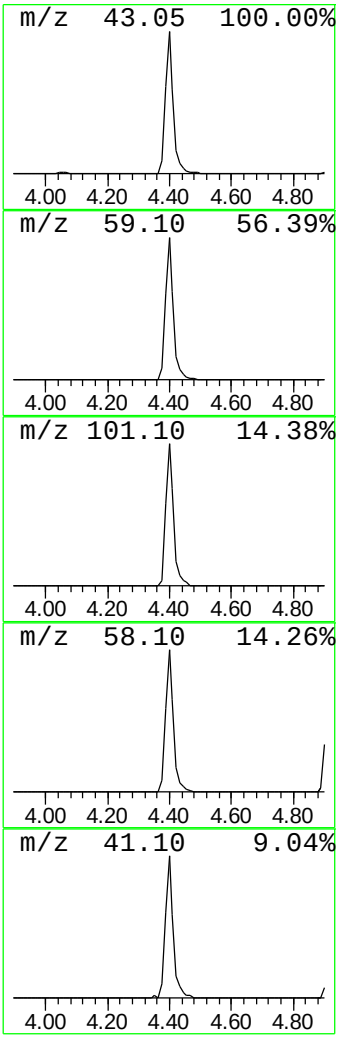
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	48.63 ng	825155	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

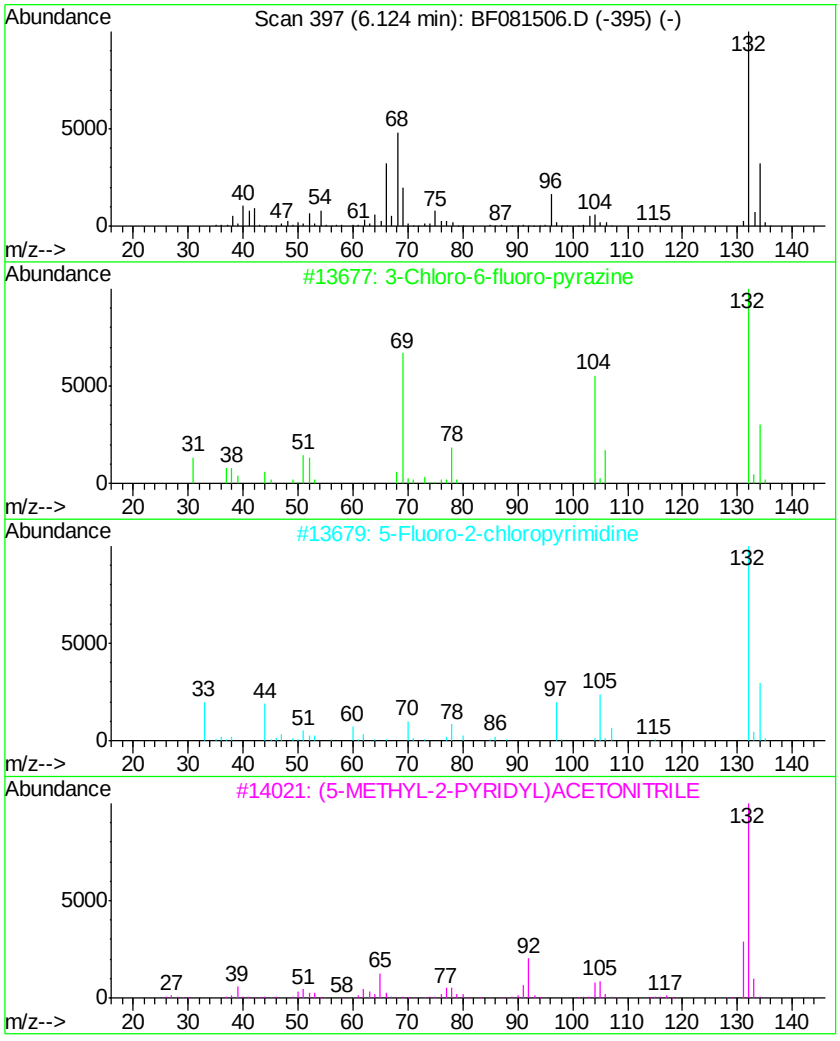
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

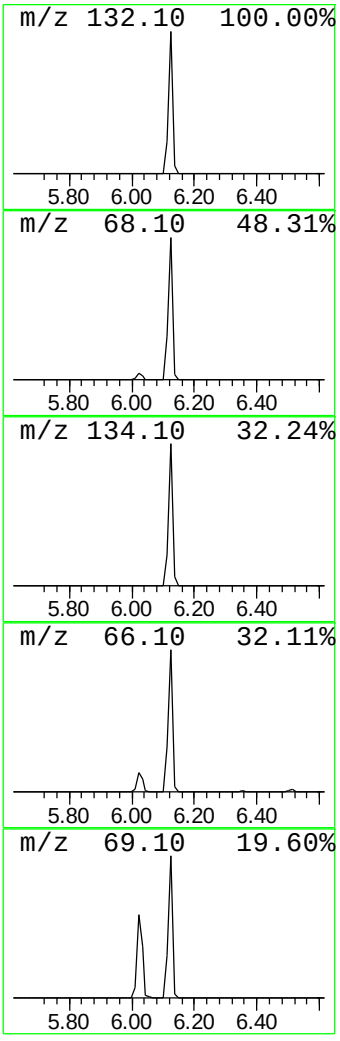
****

Peak Number 2 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	88.95 ng	1509120	1,4-Dichlorobenzene-d4	6.35

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	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

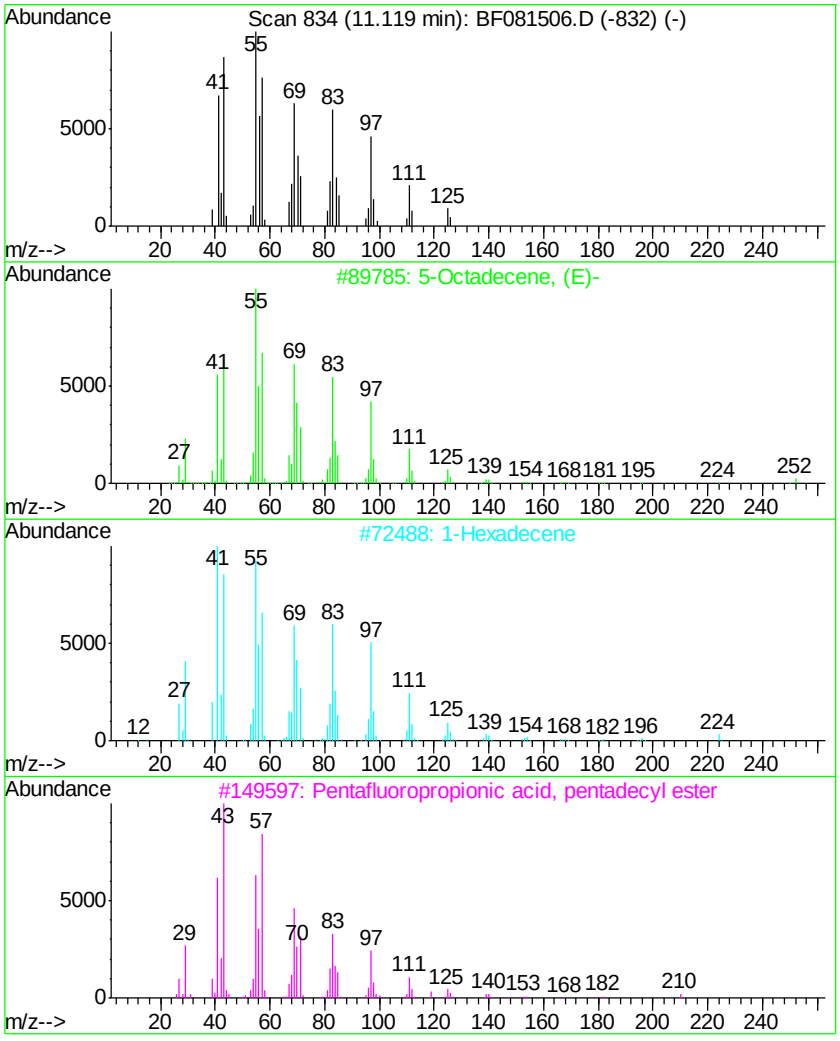
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

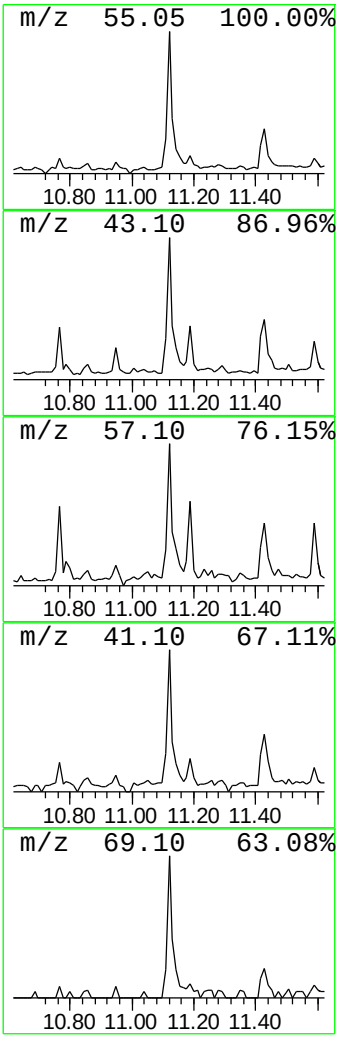
****

Peak Number 4 5-Octadecene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.12	6.61 ng	128525	Phenanthrene-d10	10.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2	1-Hexadecene	224	C16H32	000629-73-2	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	91
4	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

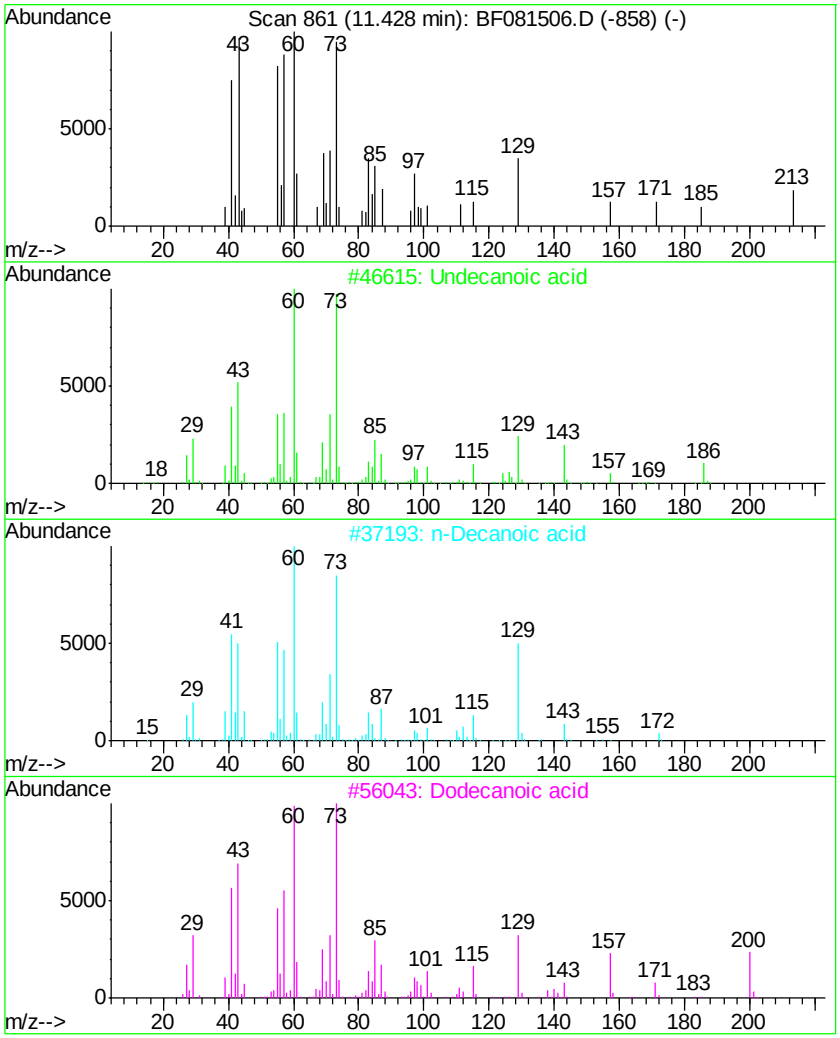
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

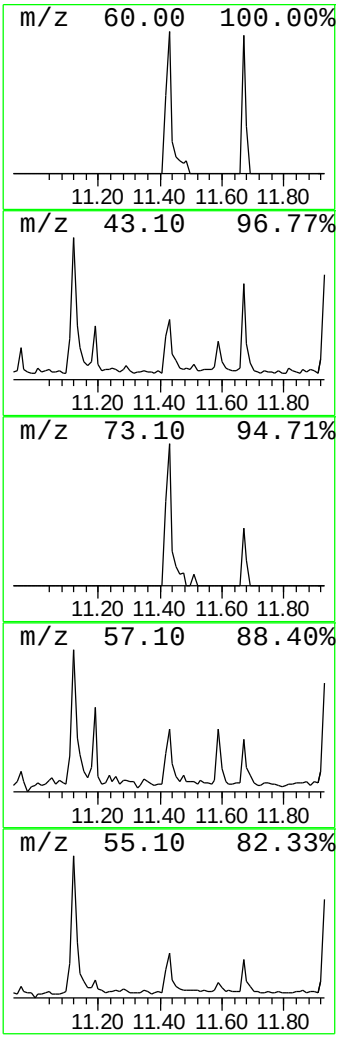
****

Peak Number 5 Undecanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	3.18 ng	61787	Phenanthrene-d10	10.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	59
3	Dodecanoic acid	200	C12H24O2	000143-07-7	59
4	.alpha.-D-Glucopyranoside, O-.al...	504	C18H32O16	000597-12-6	38
5	Amyl Nitrite	117	C5H11NO2	000110-46-3	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

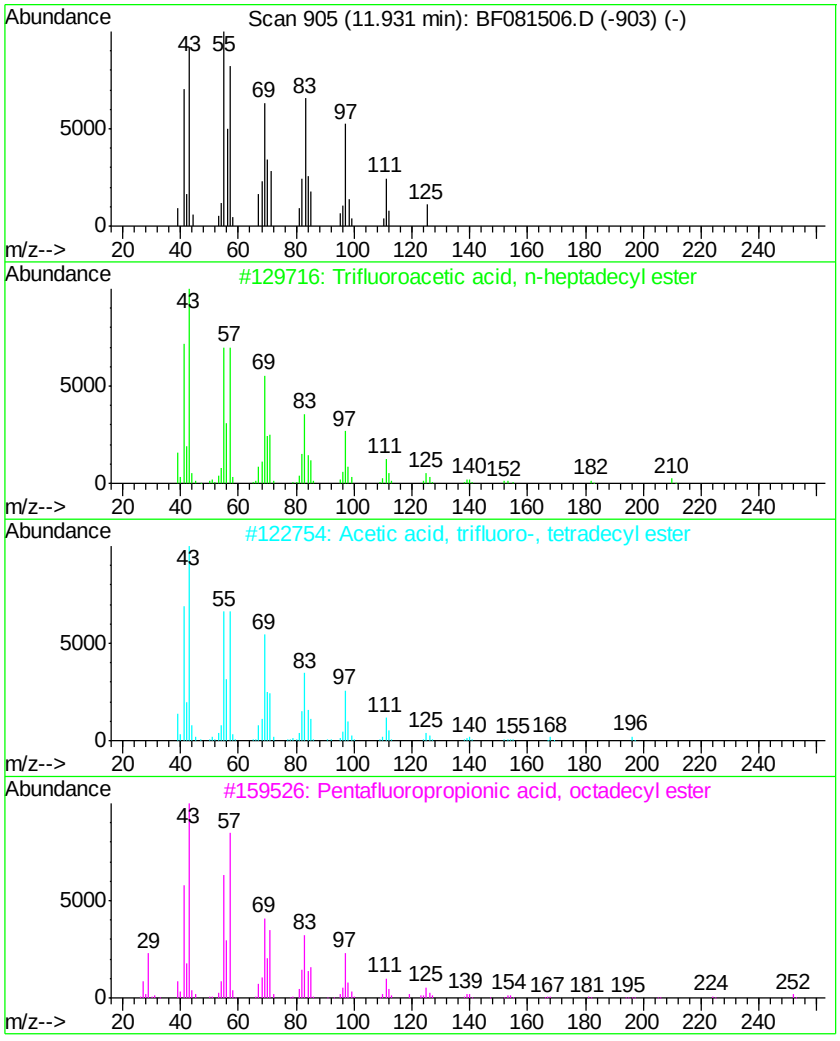
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

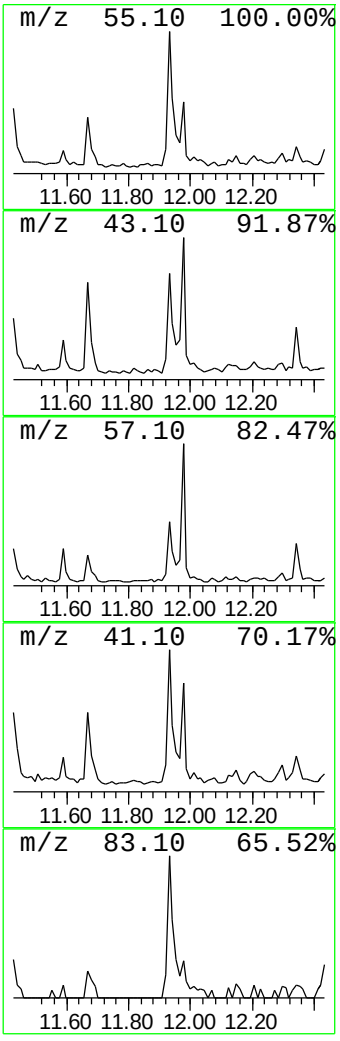
****

Peak Number 6 Trifluoroacetic acid, n-hep... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	5.48 ng	106566	Phenanthrene-d10	10.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	87
2	Acetic acid, trifluoro-, tetrade...	310	C16H29F3O2	006222-02-2	87
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	86
4	1-Tridecene	182	C13H26	002437-56-1	80
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	80





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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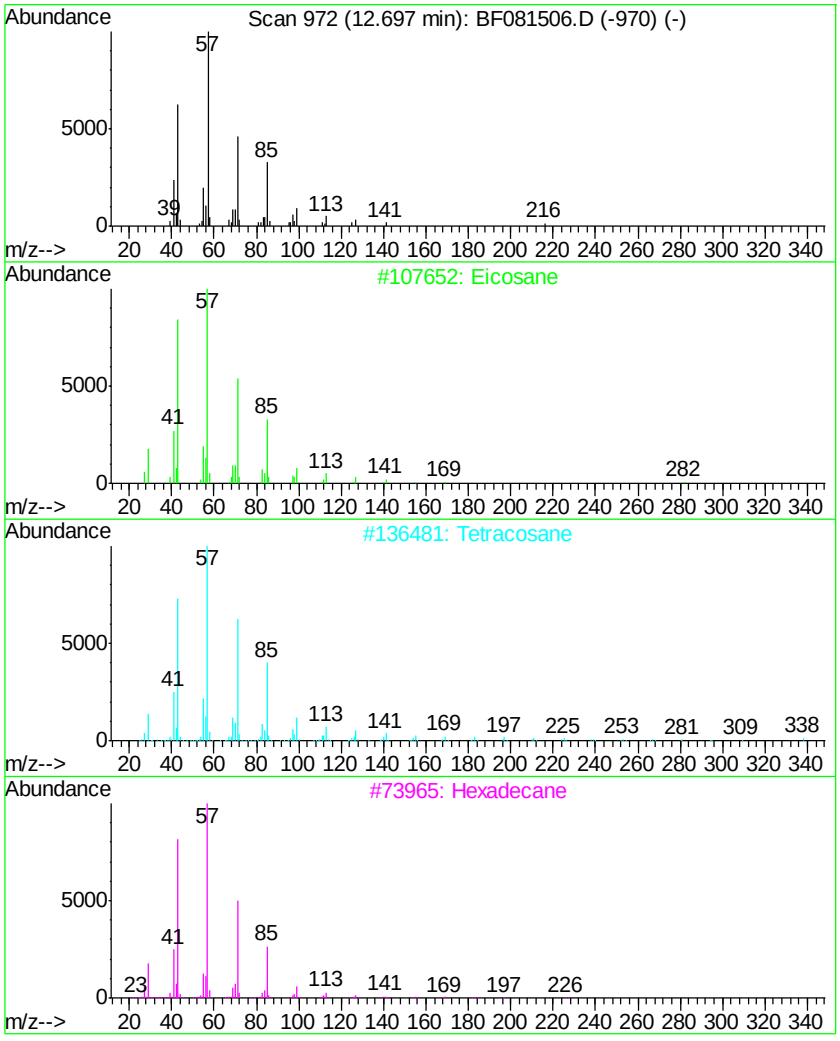
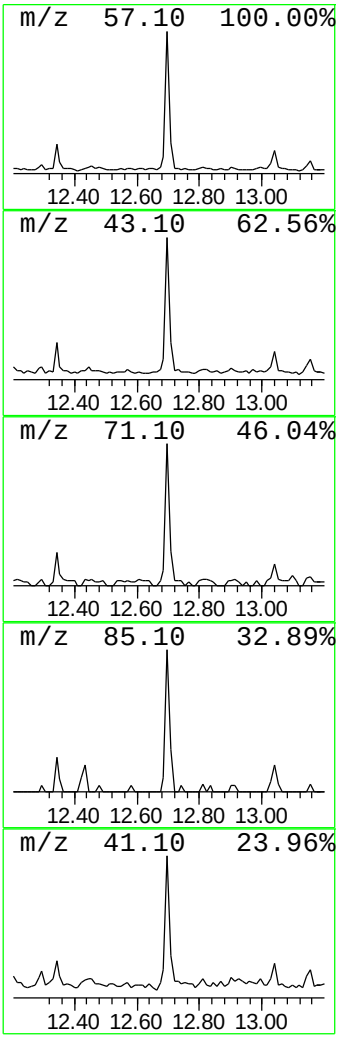
Peak Number 7 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	6.03 ng	82762	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hexadecane	226	C16H34	000544-76-3	86
4	Pentadecane	212	C15H32	000629-62-9	80
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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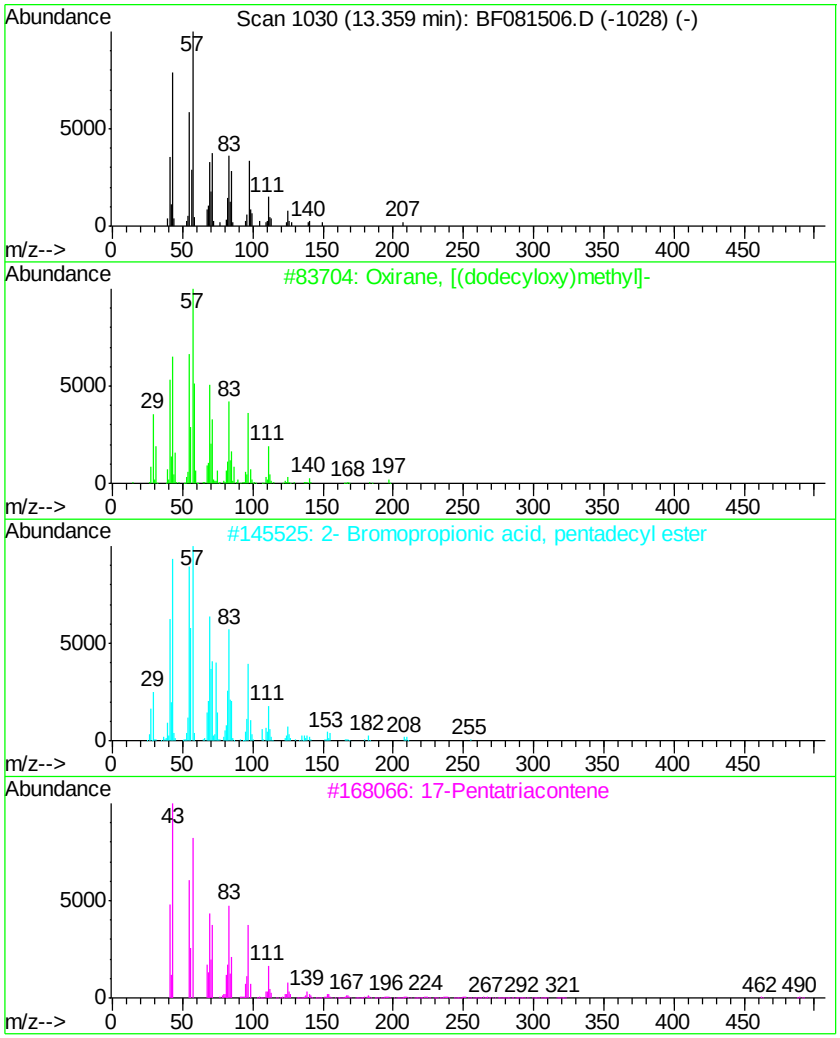
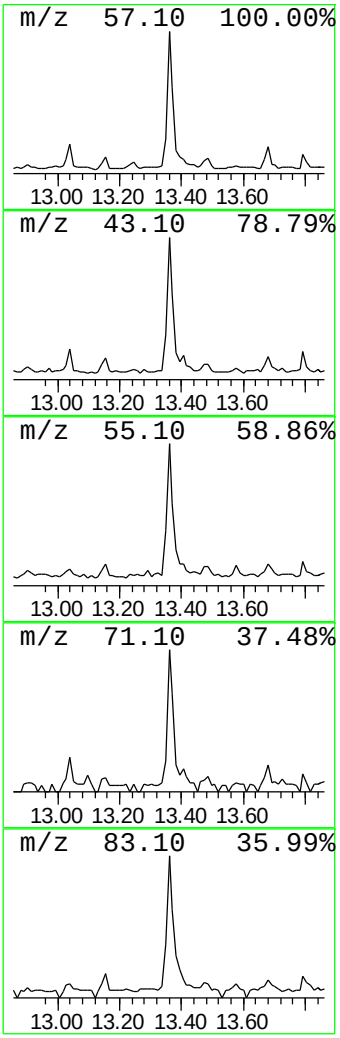
Peak Number 8 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	12.65 ng	173635	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	80
2	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	72
3	17-Pentatriacontene	491	C35H70	006971-40-0	72
4	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	72
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	62





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

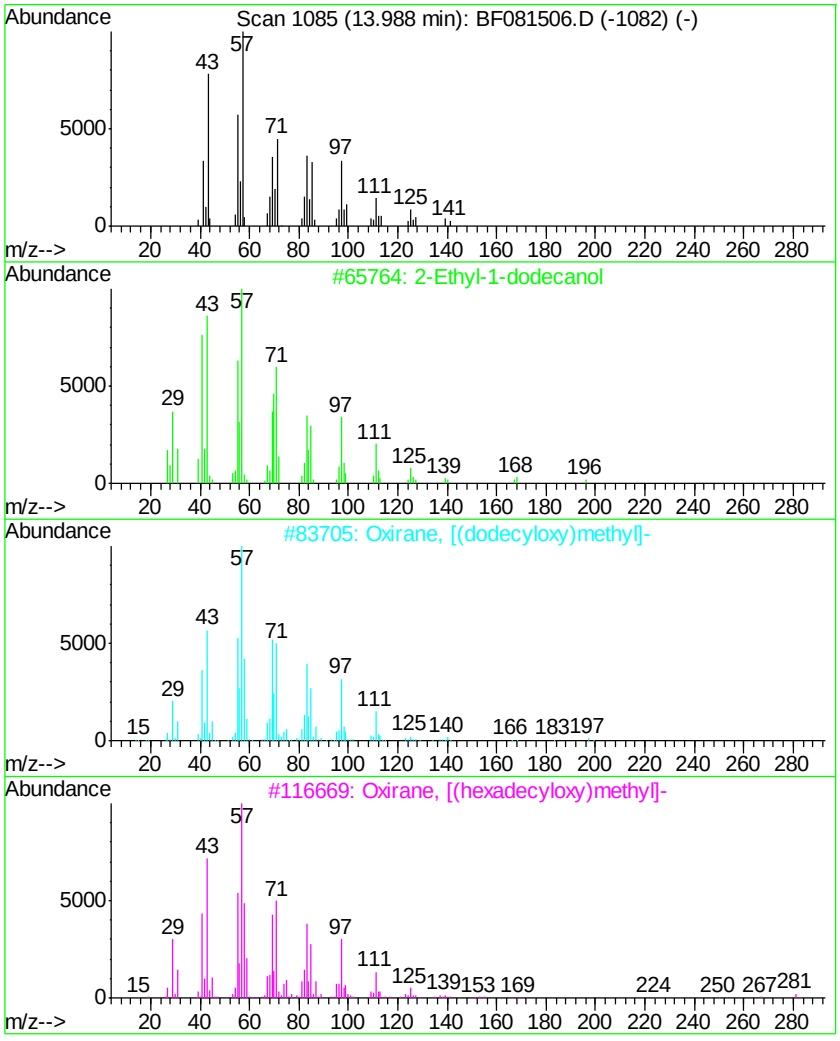
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

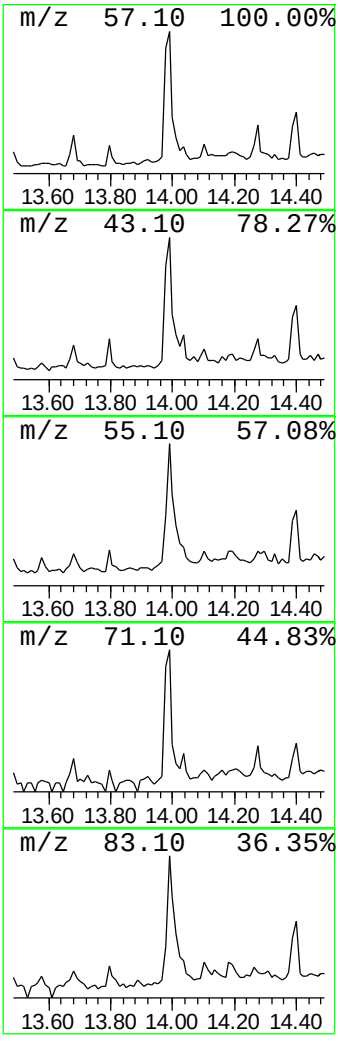
****

Peak Number 9 2-Ethyl-1-dodecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	9.11 ng	125054	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	90
2	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	80
3	Oxirane, [(hexadecyloxy)methyl]-	298	C19H38O2	015965-99-8	80
4	1-Docosene	308	C22H44	001599-67-3	70
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	62





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Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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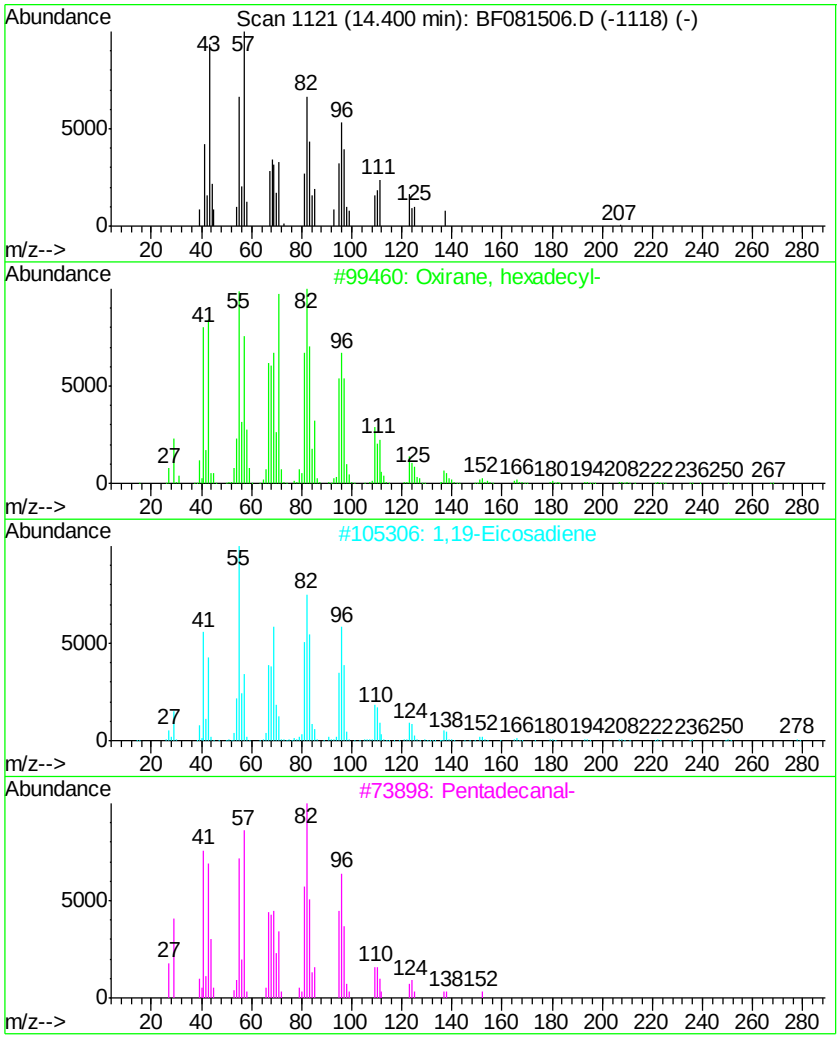
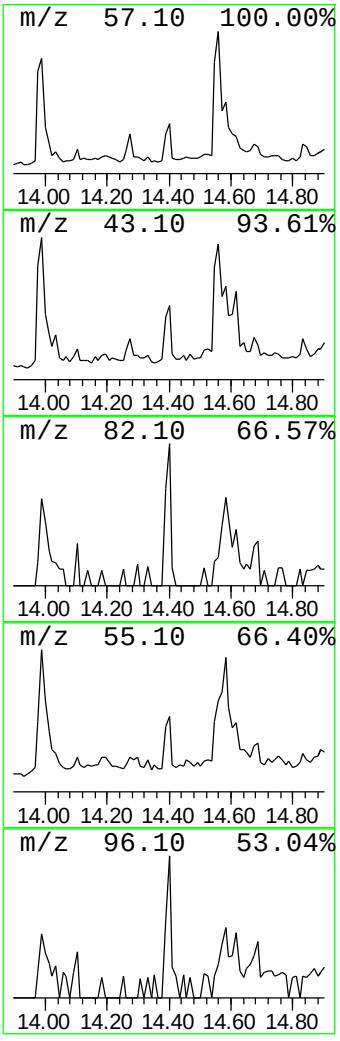
Peak Number 10 Oxirane, hexadecyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	4.32 ng	51550	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	78
2	1,19-Eicosadiene	278	C20H38	014811-95-1	72
3	Pentadecanal-	226	C15H30O	002765-11-9	64
4	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	58
5	Tetradecanal	212	C14H28O	000124-25-4	50





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ALS Vial : 81 Sample Multiplier: 1

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ClientSampleId : NCCWS

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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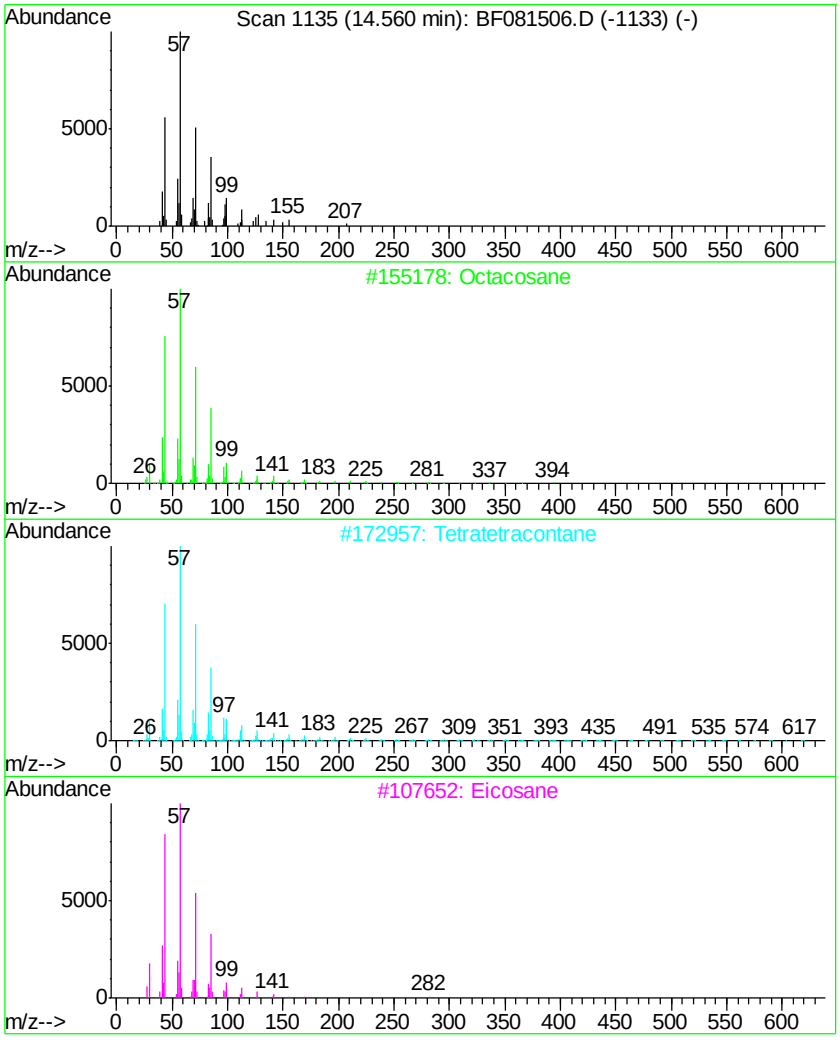
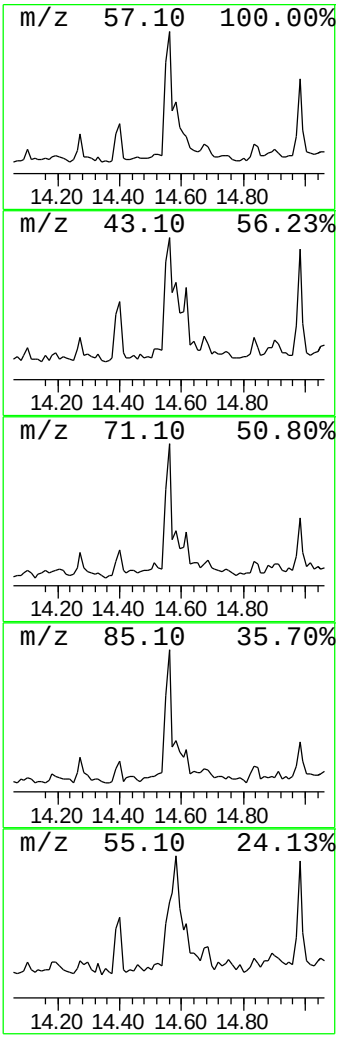
Peak Number 11 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	14.21 ng	169482	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Eicosane	282	C20H42	000112-95-8	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Hexatriacontane	507	C36H74	000630-06-8	87





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Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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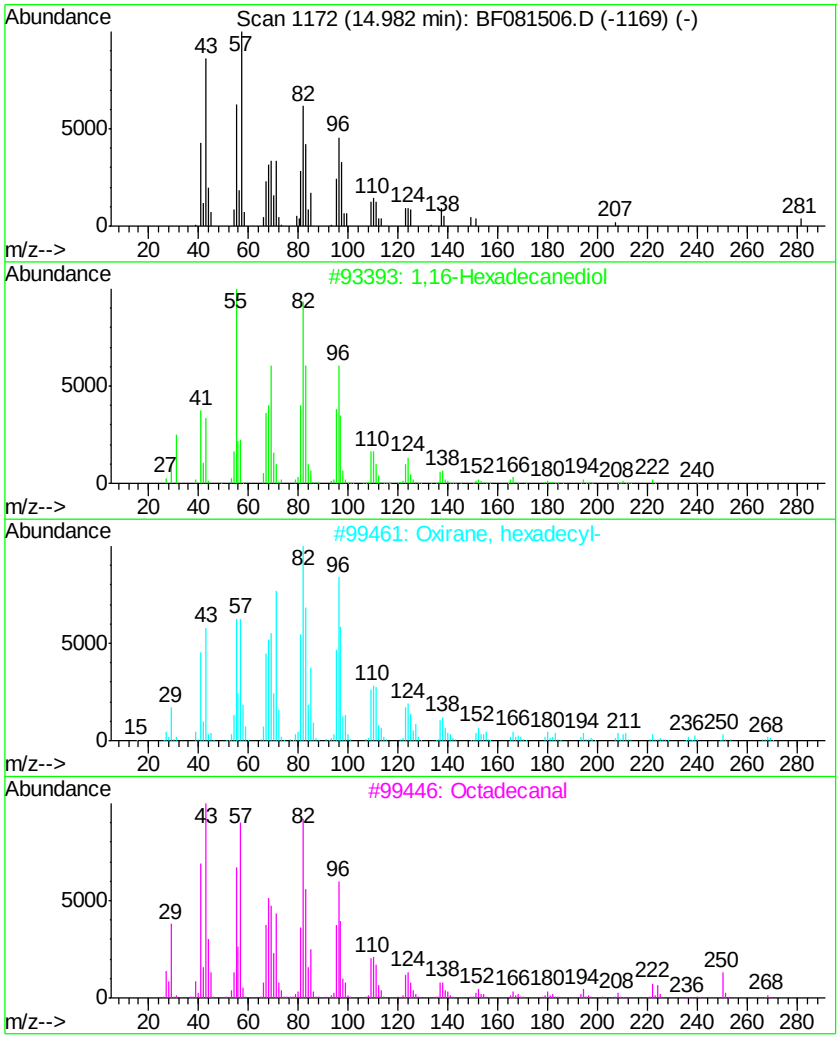
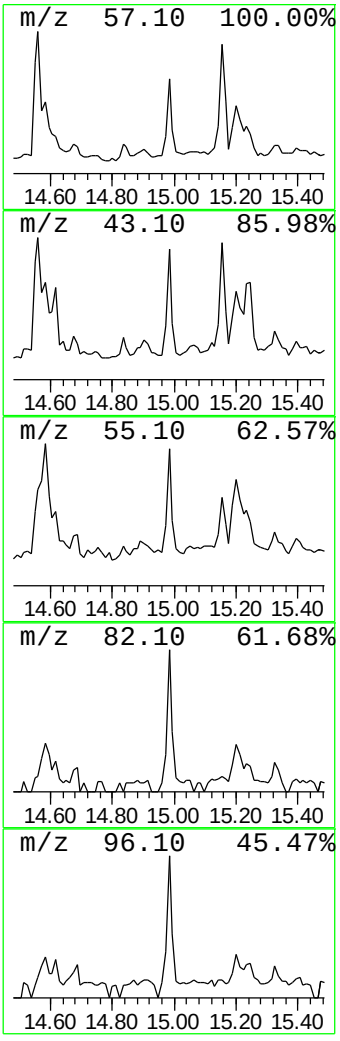
Peak Number 12 1,16-Hexadecanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	7.08 ng	84383	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Octadecanal	268	C18H36O	000638-66-4	91
4	1,19-Eicosadiene	278	C20H38	014811-95-1	91
5	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	86





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Acq On : 6 Sep 2015 13:15
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Sample : G3561-01
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ALS Vial : 81 Sample Multiplier: 1

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ClientSampleId : NCCWS

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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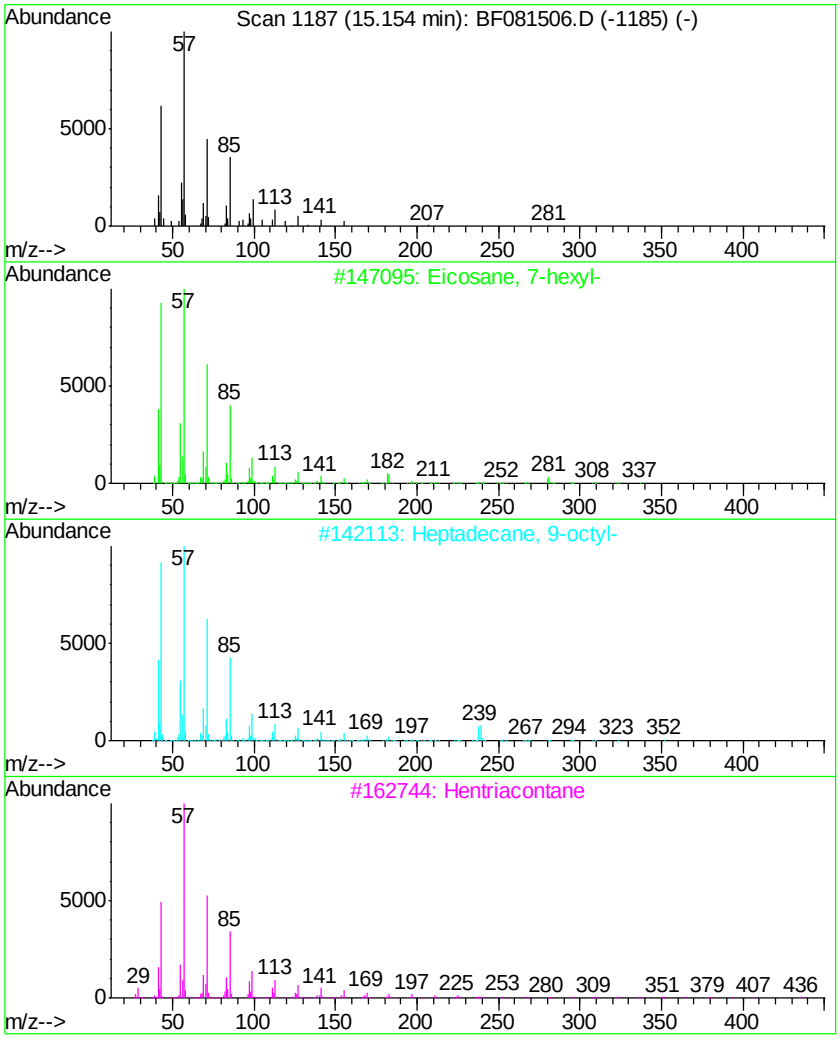
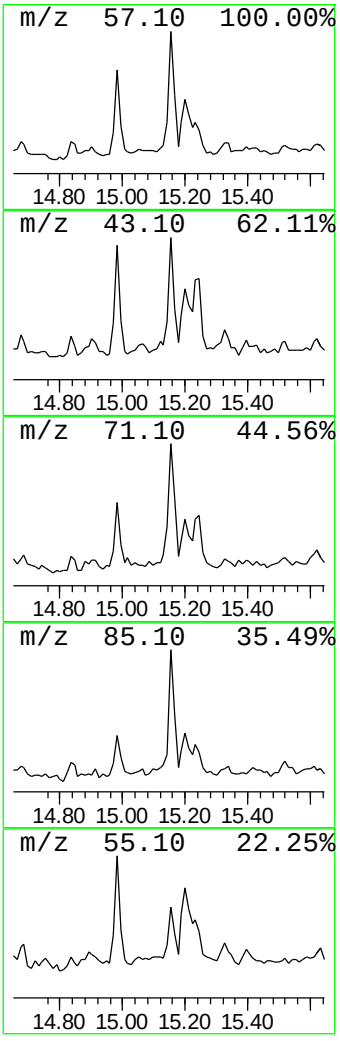
Peak Number 13 Eicosane, 7-hexyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	4.32 ng	51570	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Hentriacontane	437	C31H64	000630-04-6	90
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





Library Search Compound Report

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Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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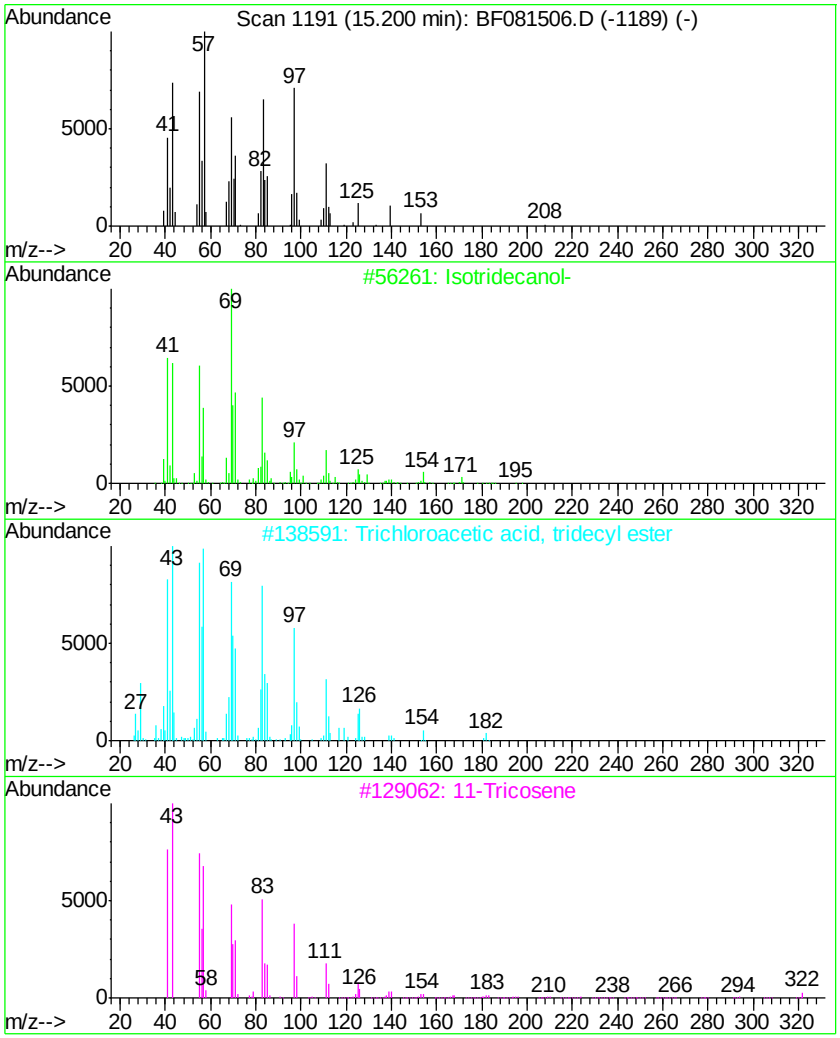
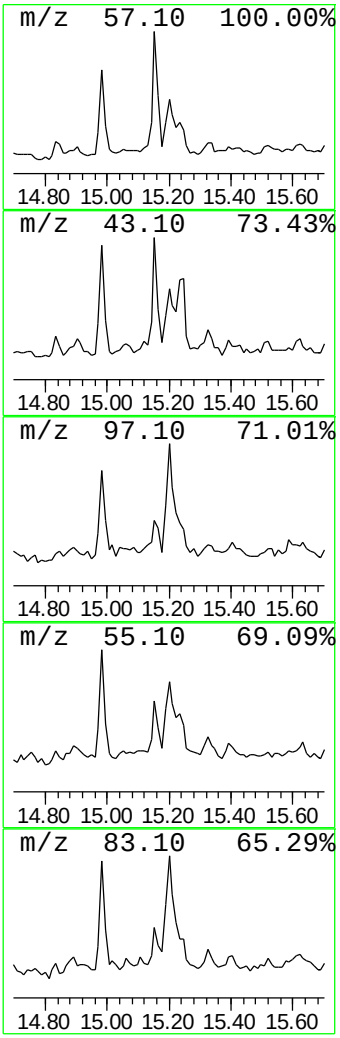
Peak Number 14 Isotridecanol- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	6.18 ng	73702	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isotridecanol-	200	C13H28O	027458-92-0	91
2	Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	87
3	11-Tricosene	322	C23H46	052078-56-5	86
4	17-Pentatriacontene	491	C35H70	006971-40-0	72
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64





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Acq On : 6 Sep 2015 13:15
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Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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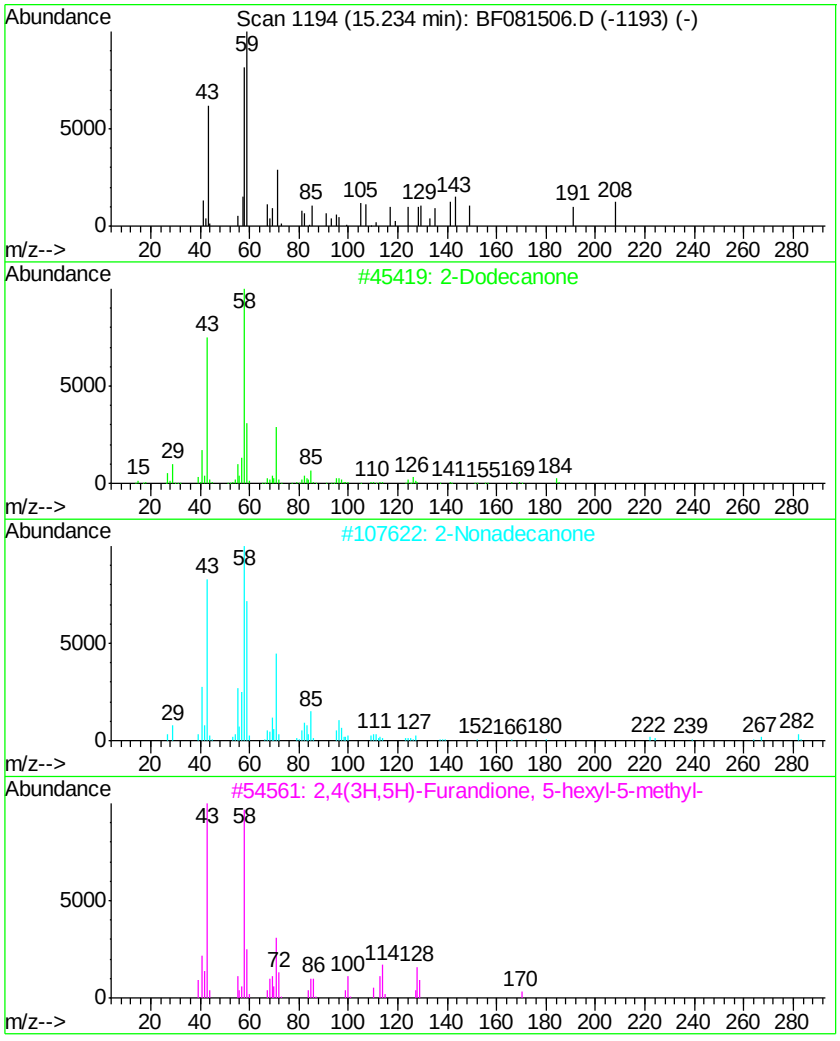
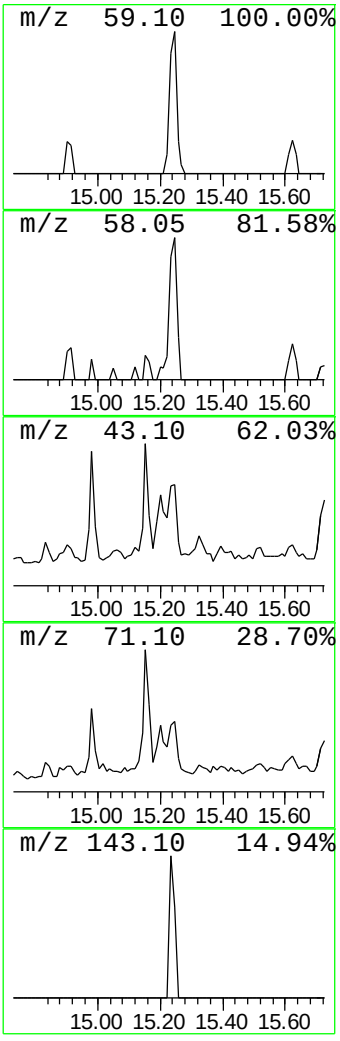
Peak Number 15 unknown15.23 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	4.02 ng	47999	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dodecanone	184	C12H24O	006175-49-1	27
2	2-Nonadecanone	282	C19H38O	000629-66-3	23
3	2,4(3H,5H)-Furandione, 5-hexyl-5...	198	C11H18O3	054852-79-8	17
4	2-Tridecanone	198	C13H26O	000593-08-8	16
5	2-Decanone	156	C10H20O	000693-54-9	12





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Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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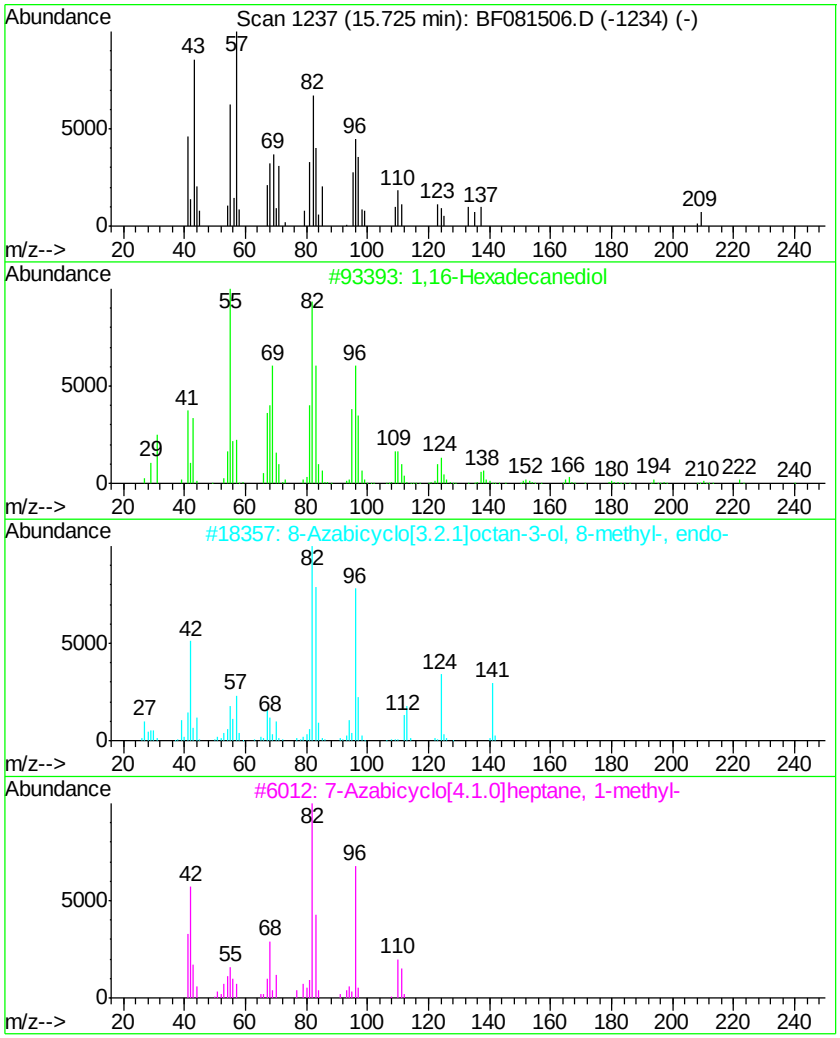
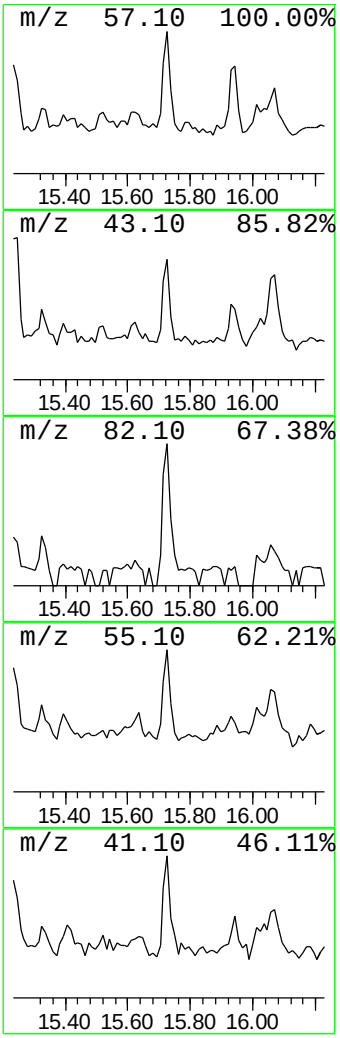
Peak Number 16 8-Azabicyclo[3.2.1]octan-3-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	5.01 ng	59733	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	74
2	8-Azabicyclo[3.2.1]octan-3-ol, 8...	141	C8H15NO	000120-29-6	50
3	7-Azabicyclo[4.1.0]heptane, 1-me...	111	C7H13N	025022-25-7	46
4	Octanenitrile	125	C8H15N	000124-12-9	43
5	1,19-Eicosadiene	278	C20H38	014811-95-1	43





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Sample : G3561-01
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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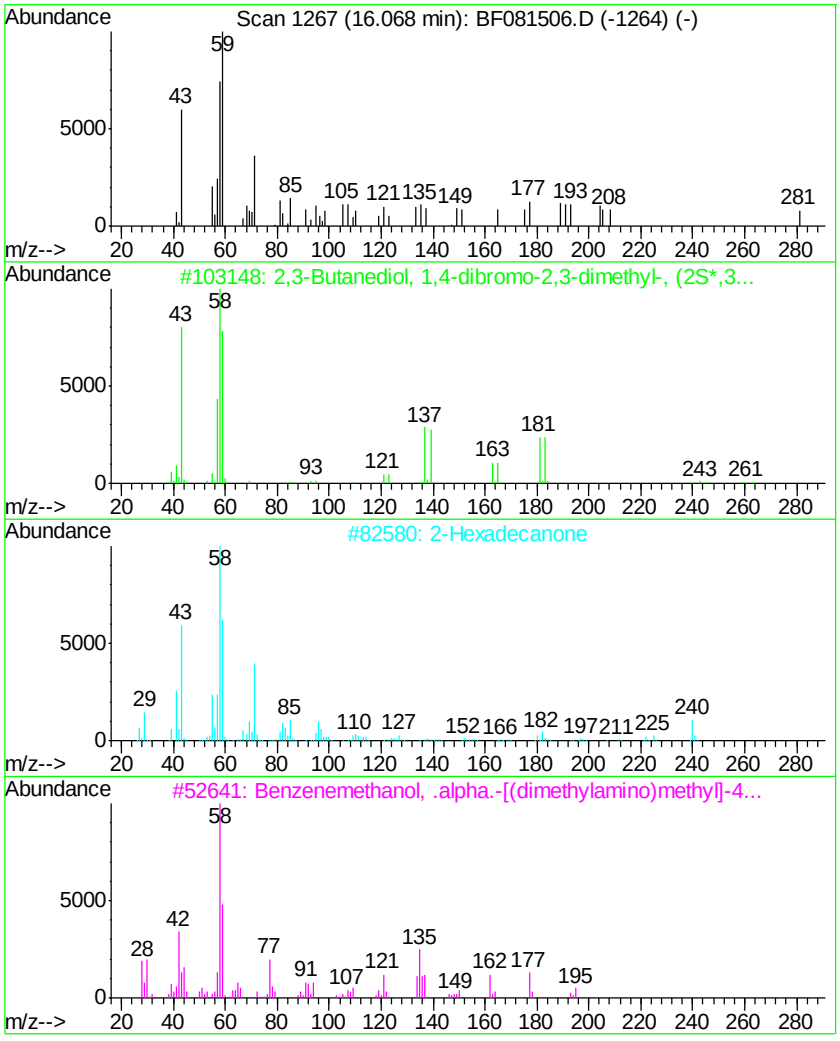
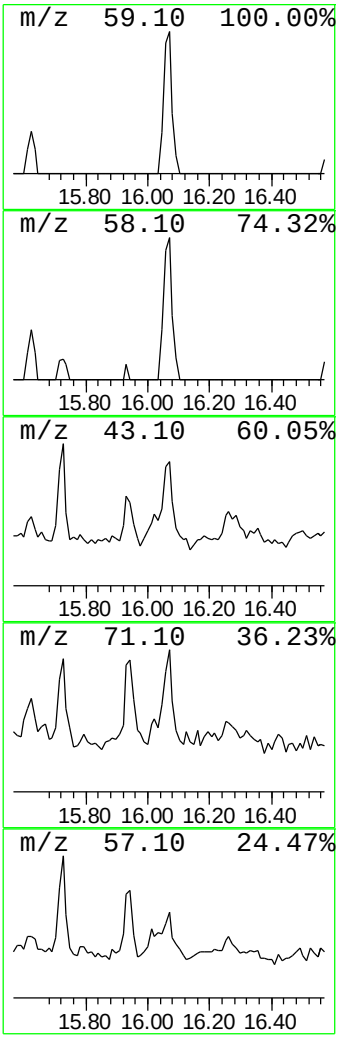
Peak Number 17 unknown16.07 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	6.14 ng	73165	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanediol, 1,4-dibromo-2,3-...	274	C6H12Br2O2	1000142-97-1	23
2	2-Hexadecanone	240	C16H32O	018787-63-8	23
3	Benzenemethanol, .alpha.-[(dimet...	195	C11H17NO2	002970-99-2	17
4	2-Ethoxyethyl trichloroacetate	234	C6H9Cl3O3	030668-97-4	16
5	2-Naphthalenemethanol, decahydro...	222	C15H26O	000473-15-4	16





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Acq On : 6 Sep 2015 13:15
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Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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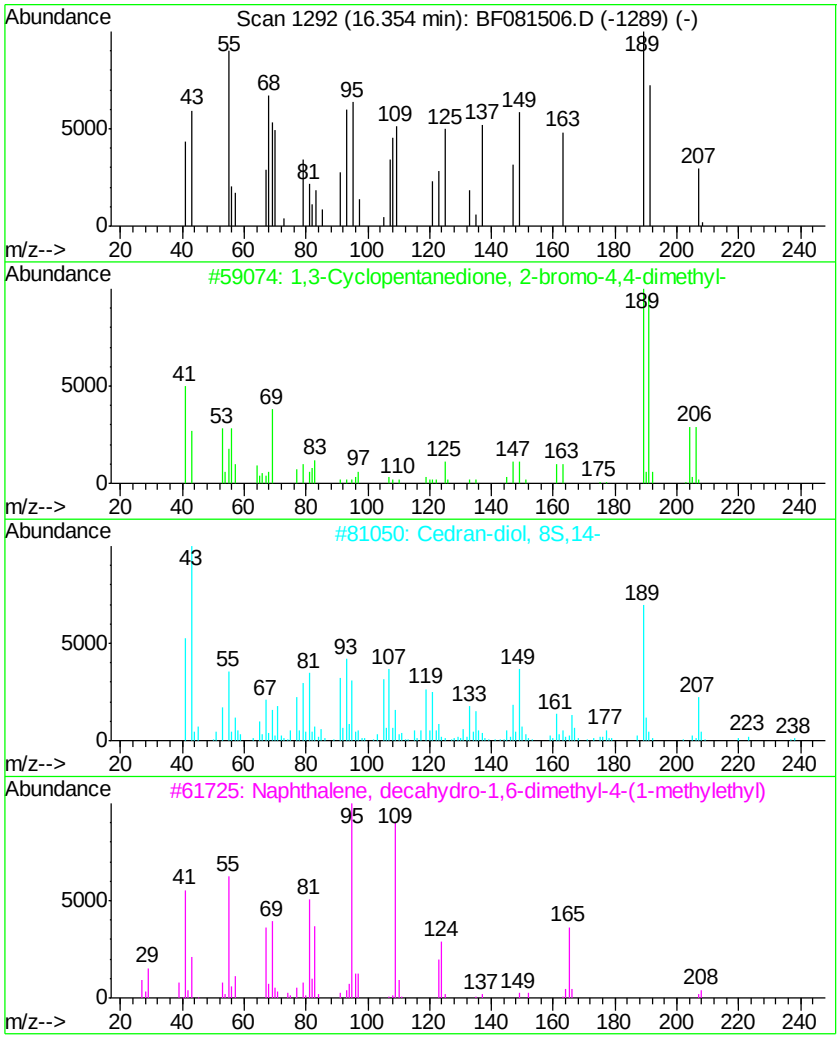
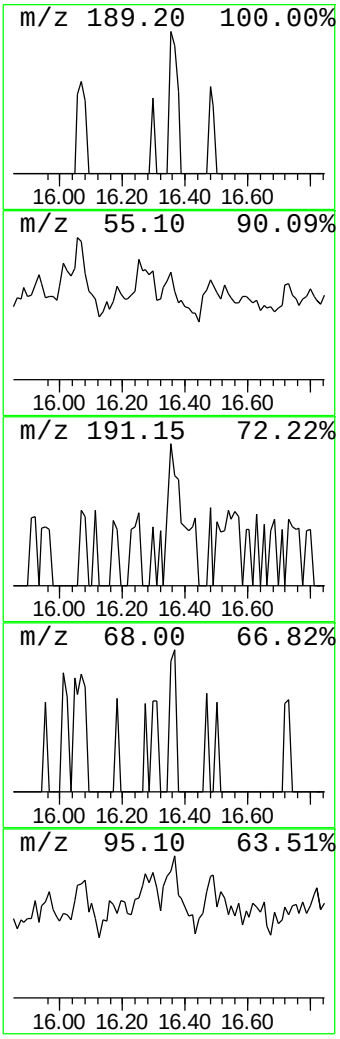
Peak Number 18 unknown16.35 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	3.33 ng	39705	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-bromo-4...	204	C7H9BrO2	057157-02-5	27
2	Cedran-diol, 8S,14-	238	C15H26O2	062600-05-9	16
3	Naphthalene, decahydro-1,6-dimet...	208	C15H28	034315-85-0	10
4	Cyclohexaneacetonitrile, 2-oxo-	137	C8H11NO	042185-27-3	9
5	Toluene, 4-chloro-2-fluoro-5-nitro-	189	C7H5ClFNO2	018349-11-6	9





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Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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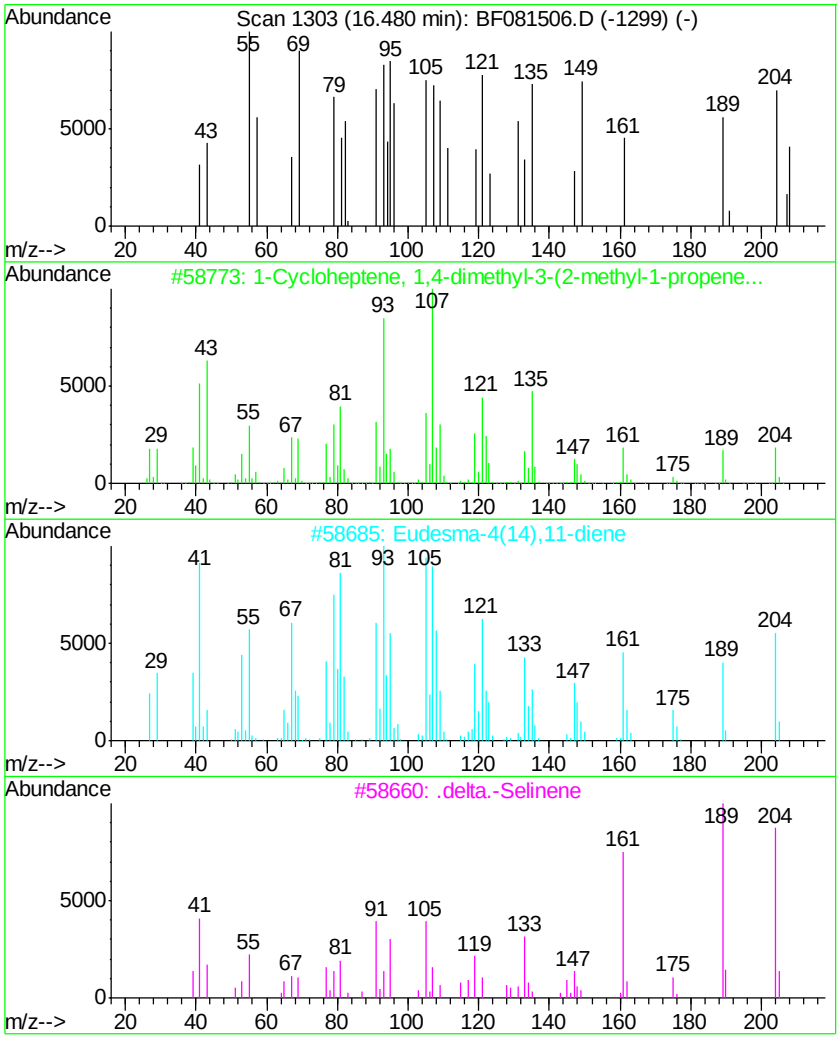
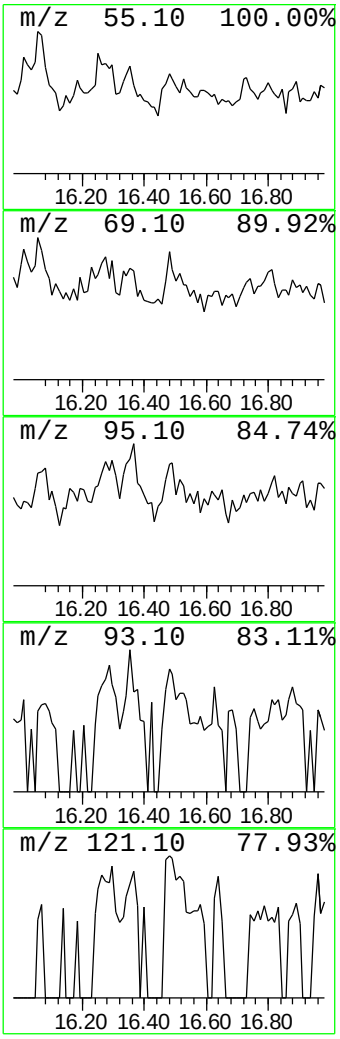
Peak Number 19 1-Cycloheptene, 1,4-dimethy... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	3.89 ng	46341	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Cycloheptene, 1,4-dimethyl-3-(...	204	C15H24	1000159-38-6	55
2	Eudesma-4(14),11-diene	204	C15H24	1000152-04-3	47
3	.delta.-Selinene	204	C15H24	028624-23-9	43
4	Longifolene-(V4)	204	C15H24	061262-67-7	42
5	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	41





Library Search Compound Report

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Sample : G3561-01
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Instrument : BNA_F
ClientSampleId : NCCWS

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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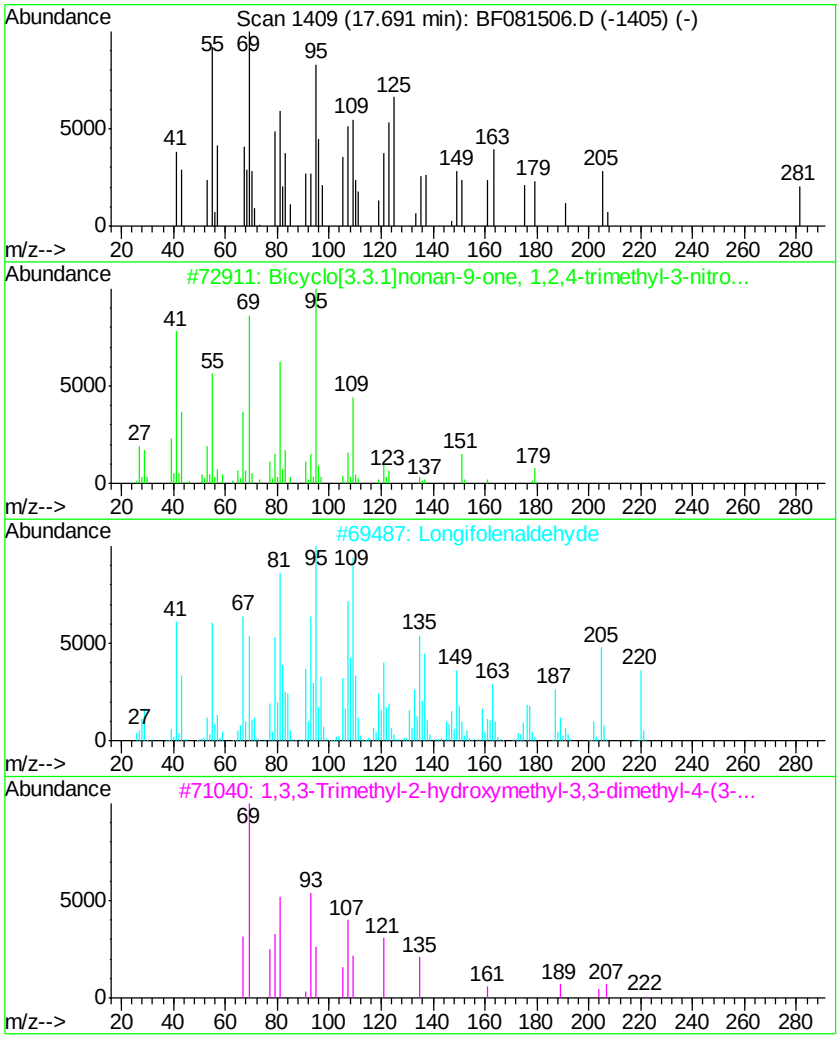
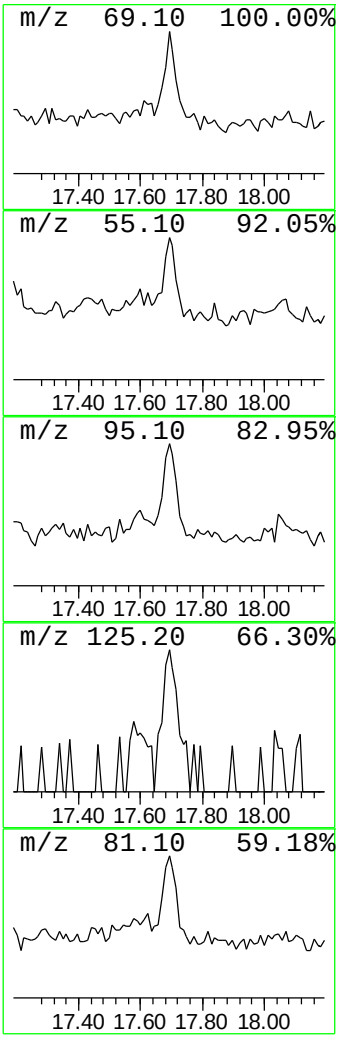
Peak Number 20 unknown17.69 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.69	6.64 ng	79242	Perylene-d12	14.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.3.1]nonan-9-one, 1,2,4...	225	C12H19NO3	129967-65-3	38
2	Longifolenaldehyde	220	C15H24O	019890-84-7	22
3	1,3,3-Trimethyl-2-hydroxymethyl-...	222	C15H26O	1000144-10-7	22
4	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	14
5	8,10-Undecadiene-3,7-dione, 4-(a...	280	C16H24O4	088354-63-6	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081506.D
Acq On : 6 Sep 2015 13:15
Operator : UM/IZ
Sample : G3561-01
Misc :
ALS Vial : 81 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NCCWS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.40	48.6	ng	825155	1	6.35	339337	20.0
unknown6.12	6.12	89.0	ng	1509120	1	6.35	339337	20.0
5-Octadecene, (E)-	11.12	6.6	ng	128525	4	10.84	388880	20.0
Undecanoic acid	11.43	3.2	ng	61787	4	10.84	388880	20.0
Trifluoroacetic a...	11.93	5.5	ng	106566	4	10.84	388880	20.0
Eicosane	12.70	6.0	ng	82762	5	13.45	274520	20.0
Oxirane, [(dodecy...	13.36	12.7	ng	173635	5	13.45	274520	20.0
2-Ethyl-1-dodecanol	13.99	9.1	ng	125054	5	13.45	274520	20.0
Oxirane, hexadecyl-	14.40	4.3	ng	51550	6	14.77	238505	20.0
Octacosane	14.56	14.2	ng	169482	6	14.77	238505	20.0
1,16-Hexadecanediol	14.98	7.1	ng	84383	6	14.77	238505	20.0
Eicosane, 7-hexyl-	15.15	4.3	ng	51570	6	14.77	238505	20.0
Isotridecanol-	15.20	6.2	ng	73702	6	14.77	238505	20.0
unknown15.23	15.23	4.0	ng	47999	6	14.77	238505	20.0
8-Azabicyclo[3.2....	15.73	5.0	ng	59733	6	14.77	238505	20.0
unknown16.07	16.07	6.1	ng	73165	6	14.77	238505	20.0
unknown16.35	16.35	3.3	ng	39705	6	14.77	238505	20.0
1-Cycloheptene, 1...	16.48	3.9	ng	46341	6	14.77	238505	20.0
unknown17.69	17.69	6.6	ng	79242	6	14.77	238505	20.0