LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102604.D
Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

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	4.899	475	478	489	rVB	35246	49355	1.71%	0.164%
2	5.322	547	550	564	rBV	1597900	1709872	59.41%	5.676%
3	6.357	722	726	740	rBV	1693596	1820854	63.27%	6.044%
4	6.481	744	747	753	rVB	1860858	1753444	60.93%	5.820%
5	6.710	783	786	794	rBV	1147361	1013379	35.21%	3.364%
6	6.869	809	813	821	rVB	1139750	1111247	38.61%	3.689%
7	7.281	879	883	891	rBV	993714	1027752	35.71%	3.411%
8	7.998	1001	1005	1011	rBV	1415878	1333133	46.32%	4.425%
9	8.051	1011	1014	1016	rVV	95613	87296	3.03%	0.290%
10	8.075	1016	1018	1027	rVB8	31350	59093	2.05%	0.196%
11	8.281	1045	1053	1055	rBV6	58625	88449	3.07%	0.294%
12	8.410	1071	1075	1077	rBV	123901	110442	3.84%	0.367%
13	8.528	1092	1095	1098	rBV3	60403	57934	2.01%	0.192%
14	8.675	1117	1120	1123	rVB3	64767	84540	2.94%	0.281%
15	8.710	1123	1126	1129	rBV4	30190	41801	1.45%	0.139%
16	8.869	1150	1153	1155	rBV2	65094	78953	2.74%	0.262%
17	8.898	1155	1158	1163	rVB4	60239	77901	2.71%	0.259%
18	8.981	1169	1172	1174	rBV3	46451	51621	1.79%	0.171%
19	9.010	1174	1177	1180	rVV	305104	225582	7.84%	0.749%
20	9.069	1183	1187	1191	rBV	1731937	1490513	51.79%	4.947%
21	9.145	1196	1200	1205	rBV4	133002	183655	6.38%	0.610%
22	9.186	1205	1207	1211	rBV4	58040	73859	2.57%	0.245%
23	9.339	1230	1233	1235	rBV2	74518	86293	3.00%	0.286%
24	9.469	1249	1255	1257	rBV2	728416	822540	28.58%	2.730%
25	9.498	1257	1260	1262	rVB3	41071	41411	1.44%	0.137%
26	9.557	1266	1270	1271	rBV4	94156	111868	3.89%	0.371%
27	9.610	1276	1279	1283	rBV2	256054	308718	10.73%	1.025%
28	9.651	1283	1286	1289	rBV	255470	214447	7.45%	0.712%
29	9.686	1289	1292	1294	rBV4	74252	98479	3.42%	0.327%
30	9.716	1294	1297	1299	rBV3	152550	190724	6.63%	0.633%
31	9.751	1299	1303	1306	rVB	1531405	1355463	47.10%	4.499%
32	9.781	1306	1308	1311	rBV2	190691	148651	5.17%	0.493%
33	9.851	1318	1320	1324	rVB3	125352	106191	3.69%	0.352%
34	9.939	1332	1335	1337	rBV	248756	240321	8.35%	0.798%

LSC Area Percent Report

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Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

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

35	9.998	1342	1345	1348	rBV4	402003	444486	15.44%	1.475%
36	10.063	1353	1356	1360	rBV4	175604	285797	9.93%	0.949%
37	10.151	1368	1371	1373	rBV3	239906	273182	9.49%	0.907%
38	10.204	1377	1380	1382	rBV2	182142	224195	7.79%	0.744%
39	10.398	1409	1413	1417	rVB	1448494	1424754	49.51%	4.729%
40	10.545	1435	1438	1442	rBV2	793805	944437	32.82%	3.135%
41	10.581	1442	1444	1447	rVB4	338176	349983	12.16%	1.162%
42	10.663	1454	1458	1465	rBV	2487122	2877871	100.00%	9.552%
43	11.133	1534	1538	1544	rVB	2362355	2583007	89.75%	8.574%
44	11.239	1553	1556	1559	rBV	1333274	1483545	51.55%	4.924%
45	11.480	1594	1597	1600	rBV	858953	891605	30.98%	2.959%
46	12.463	1762	1764	1767	rVB	812795	615809	21.40%	2.044%
47	12.692	1801	1803	1810	rVB2	693579	802162	27.87%	2.663%
48	15.327	2247	2251	2254	rVB	536998	670594	23.30%	2.226%

Sum of corrected areas: 30127208

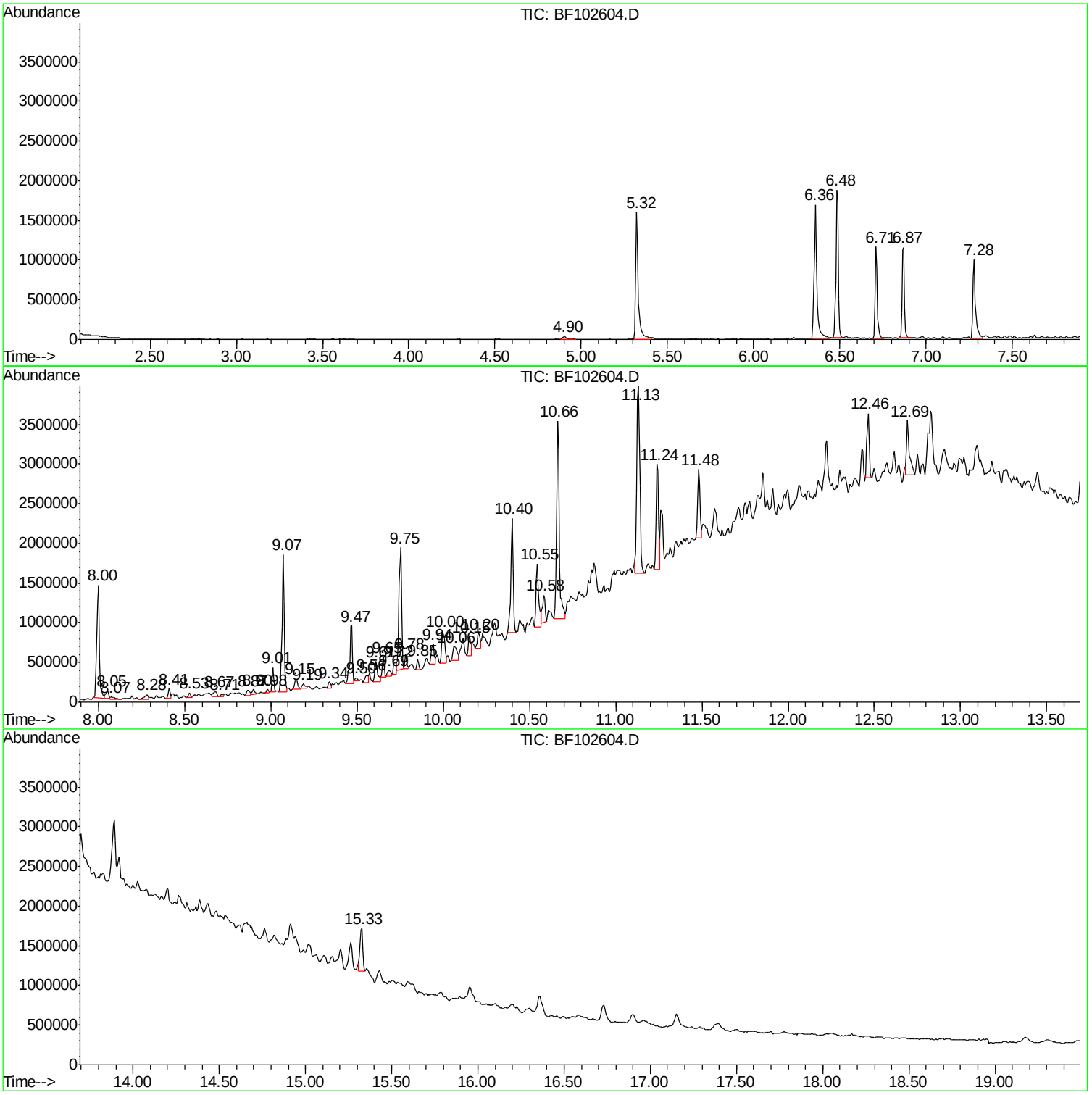
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102604.D
Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102604.D
Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

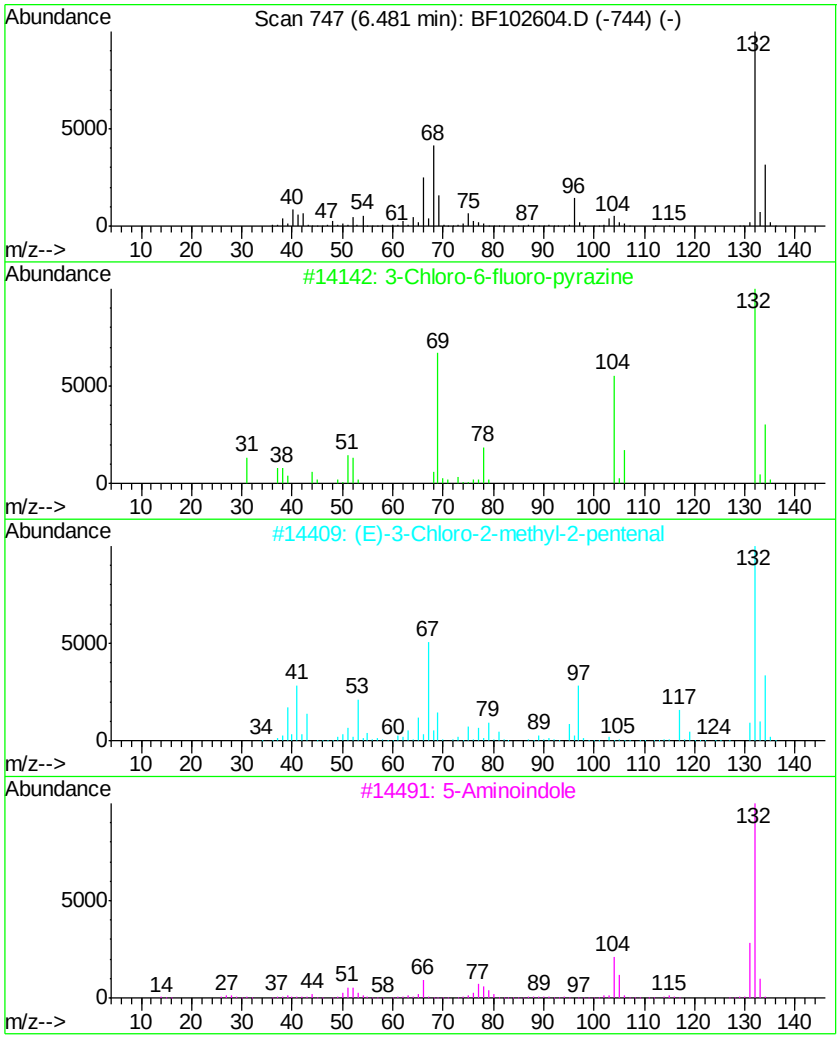
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

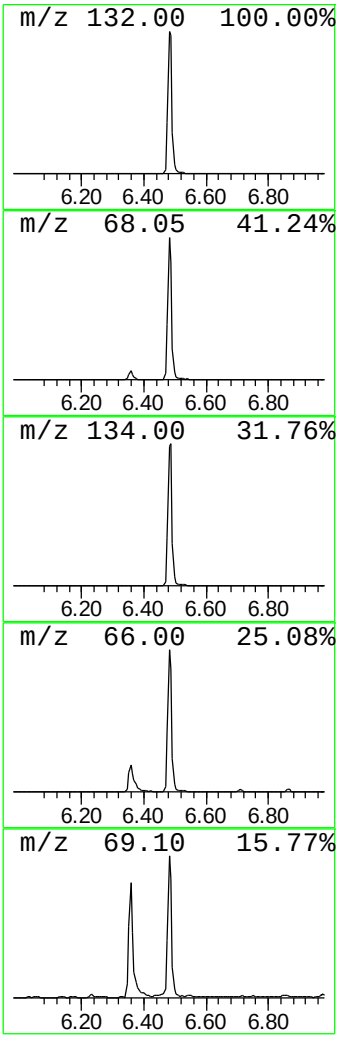
****

Peak Number 1 unknown6.48 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	34.61 ng	1753440	1,4-Dichlorobenzene-d4	6.71

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102604.D
Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

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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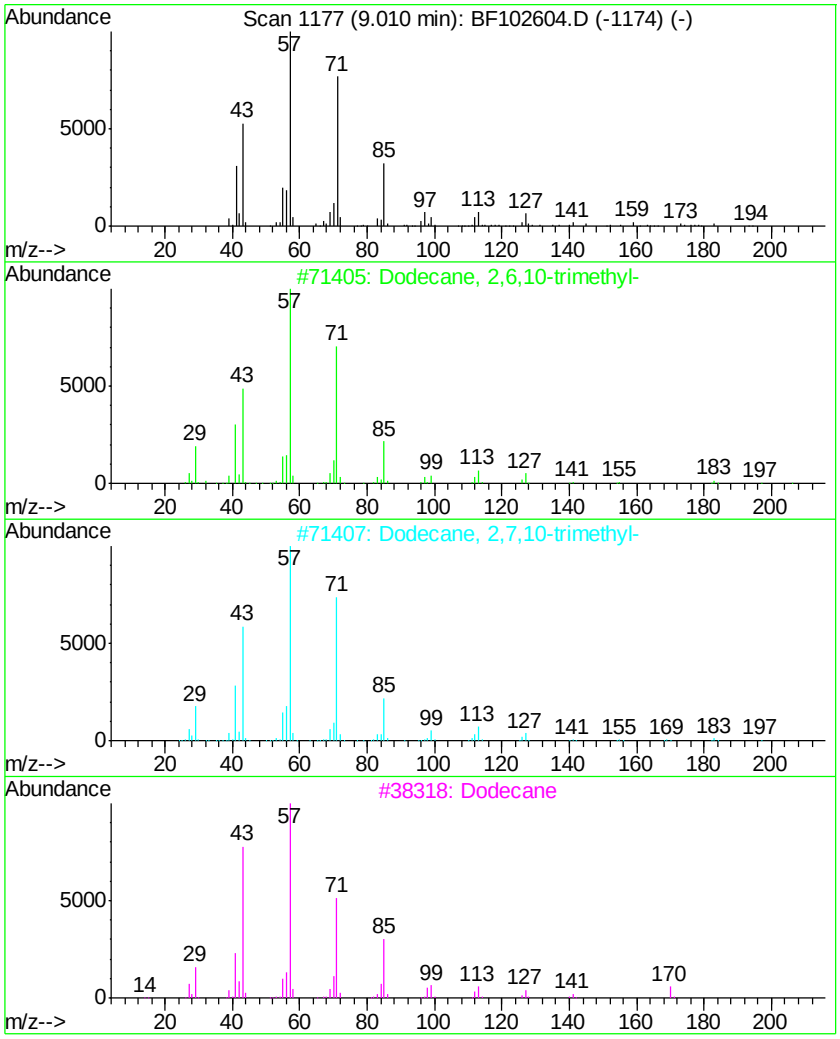
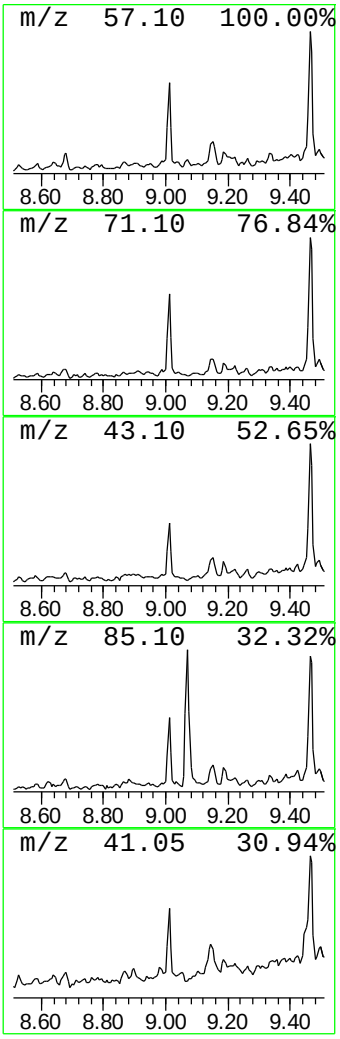
Peak Number 3 Dodecane, 2,6,10-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.01	3.33 ng	225582	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	90
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
3	Dodecane	170	C12H26	000112-40-3	78
4	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	78
5	Heptane, 3-(bromomethyl)-	192	C8H17Br	018908-66-2	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102604.D
Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

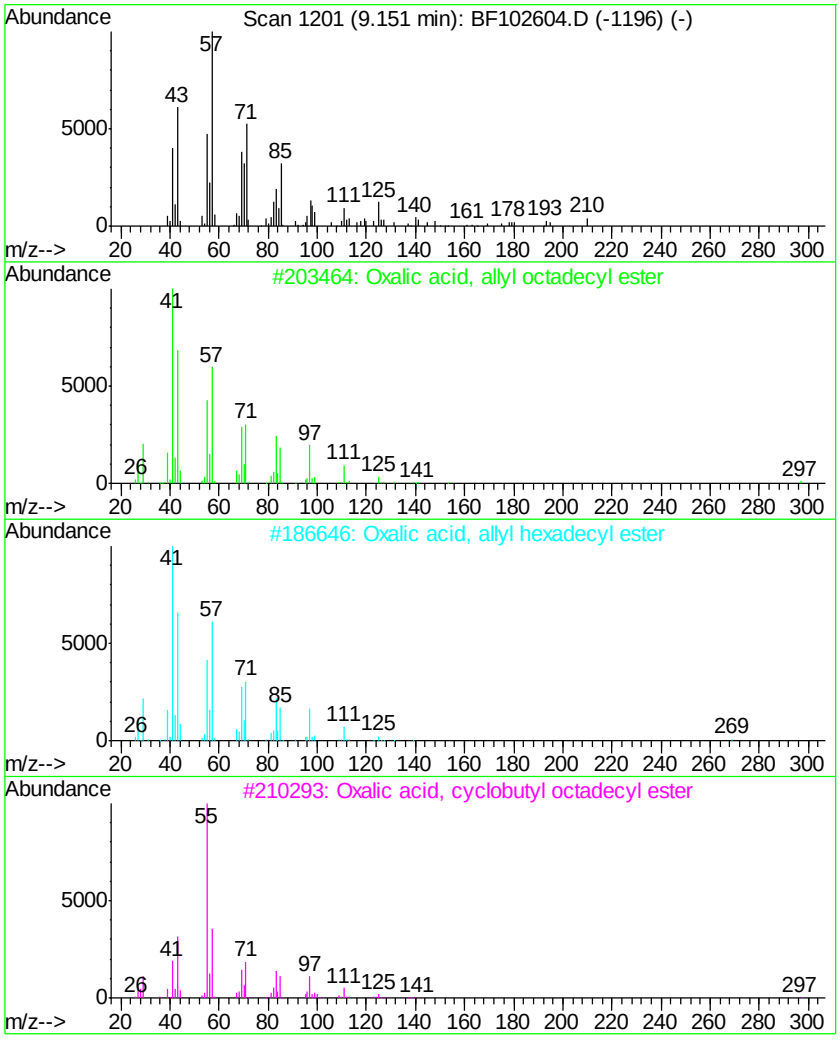
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

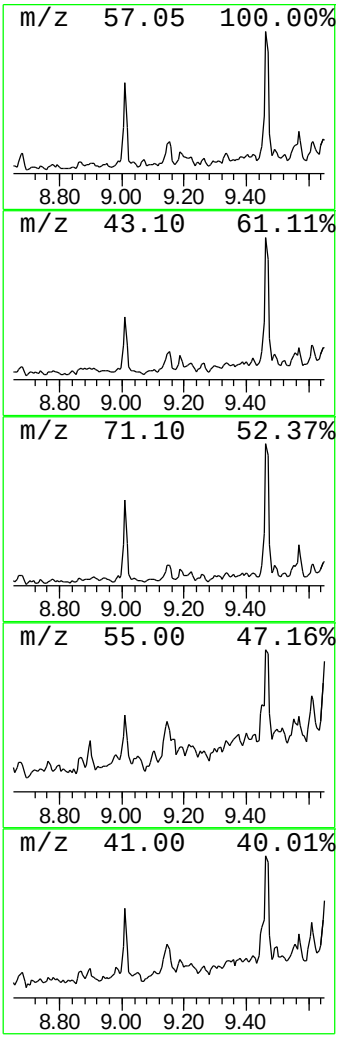
****

Peak Number 4 Oxalic acid, allyl octadecy... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.15	2.71 ng	183655	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	58
2	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	52
3	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	52
4	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	38
5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
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Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

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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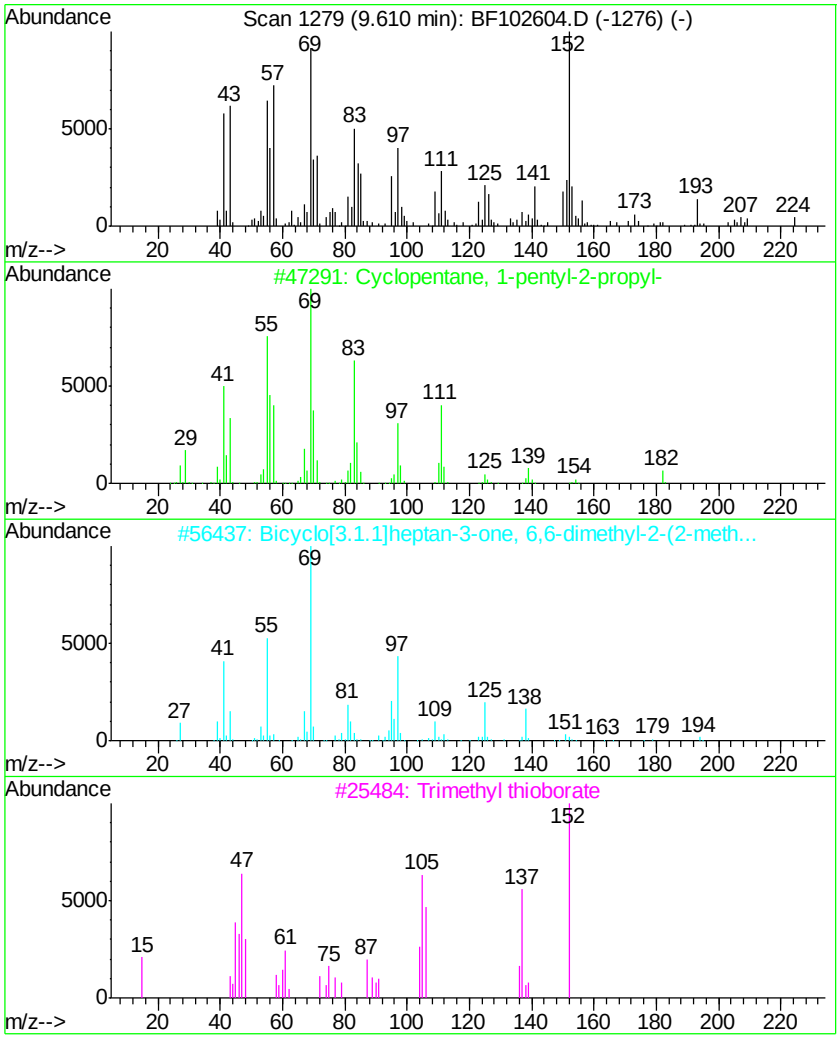
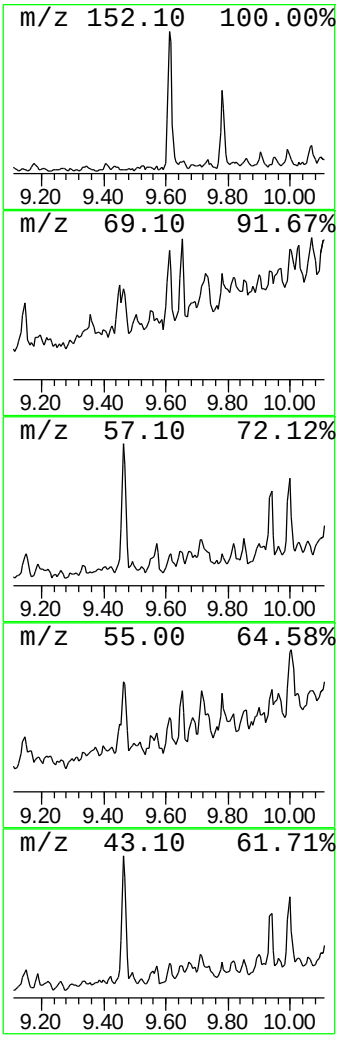
Peak Number 5 unknown9.51 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.61	4.56 ng	308718	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	38
2	Bicyclo[3.1.1]heptan-3-one, 6,6-...	194	C13H22O	1000163-97-9	30
3	Trimethyl thioborate	152	C3H9BS3	000997-49-9	25
4	Bicyclo(3.3.1)nonane-2,6-dione	152	C9H12O2	016473-11-3	25
5	Biphenylene	152	C12H8	000259-79-0	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102604.D
Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

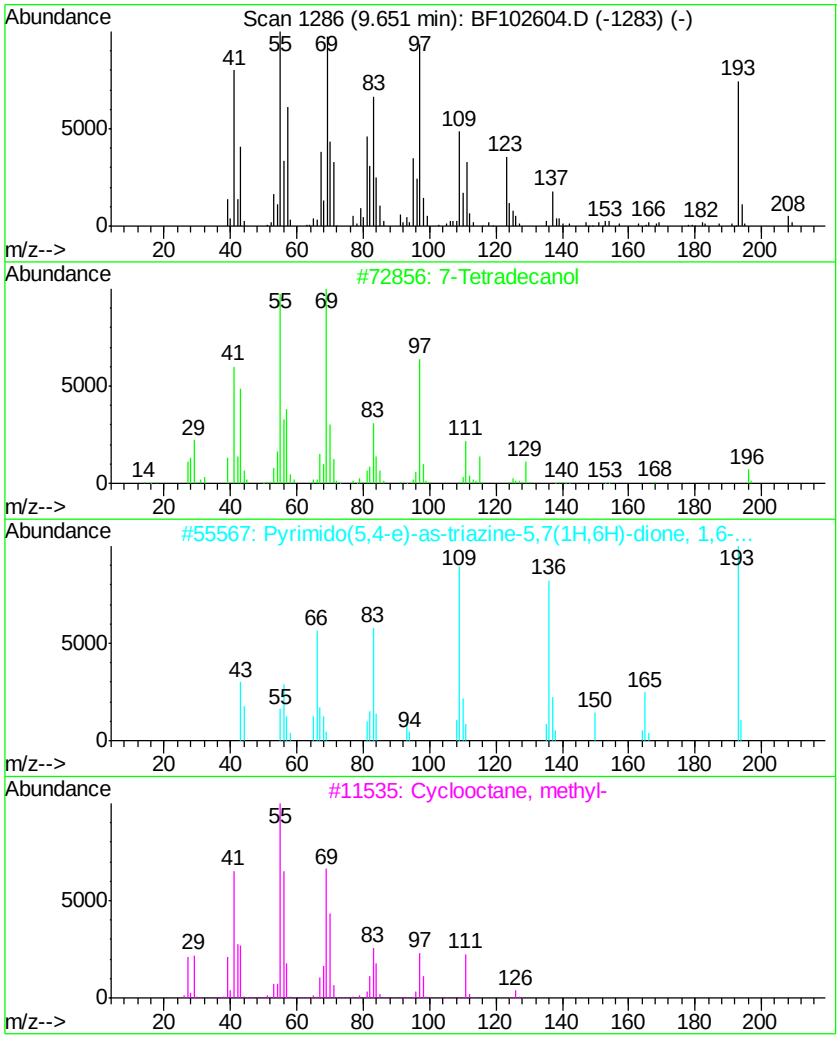
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

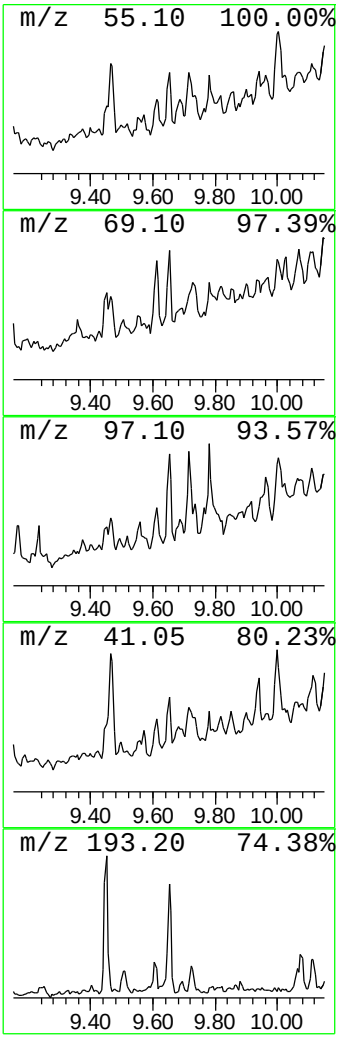
****

Peak Number 6 unknown9.65 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.65	3.16 ng	214447	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Tetradecanol	214	C14H30O	003981-79-1	38
2	Pyrimido(5,4-e)-as-triazine-5,7(...	193	C7H7N5O2	000084-82-2	25
3	Cyclooctane, methyl-	126	C9H18	001502-38-1	25
4	Crotyl methacrylate	140	C8H12O2	007376-45-6	20
5	2-Undecanethiol, 2-methyl-	202	C12H26S	010059-13-9	18





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
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Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

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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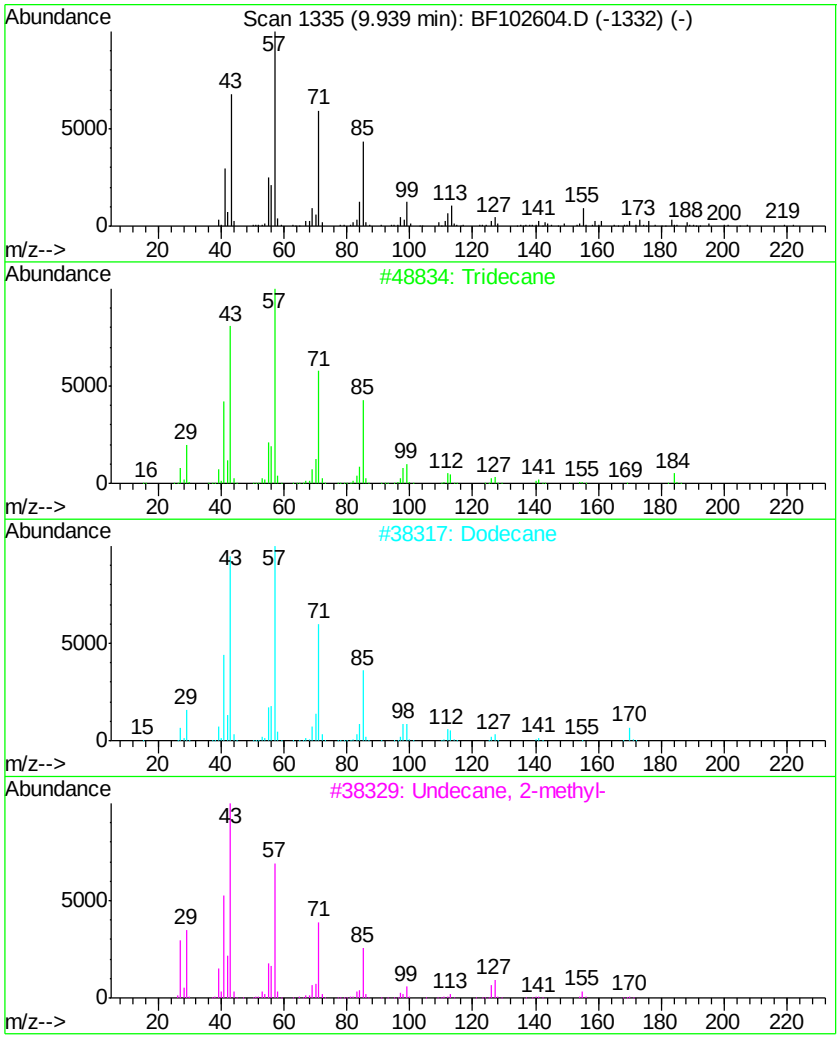
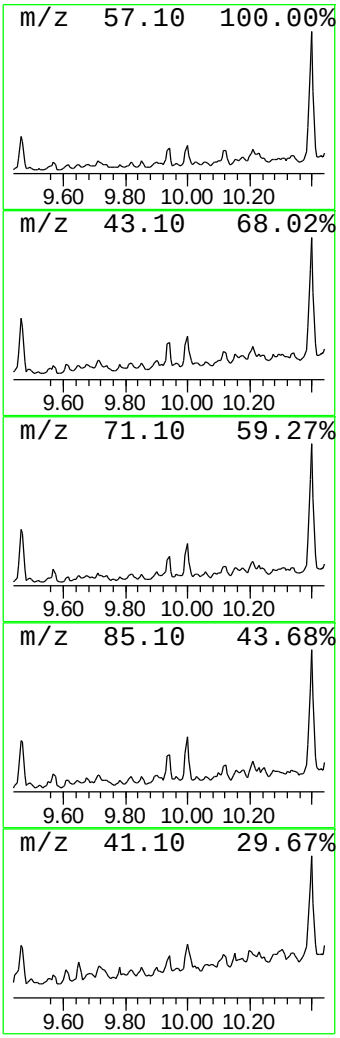
Peak Number 7 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.94	3.55 ng	240321	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Dodecane	170	C12H26	000112-40-3	74
3	Undecane, 2-methyl-	170	C12H26	007045-71-8	72
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
5	Octane, 2-methyl-	128	C9H20	003221-61-2	64





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Instrument : BNA_F
ClientSampleId : WC-16(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

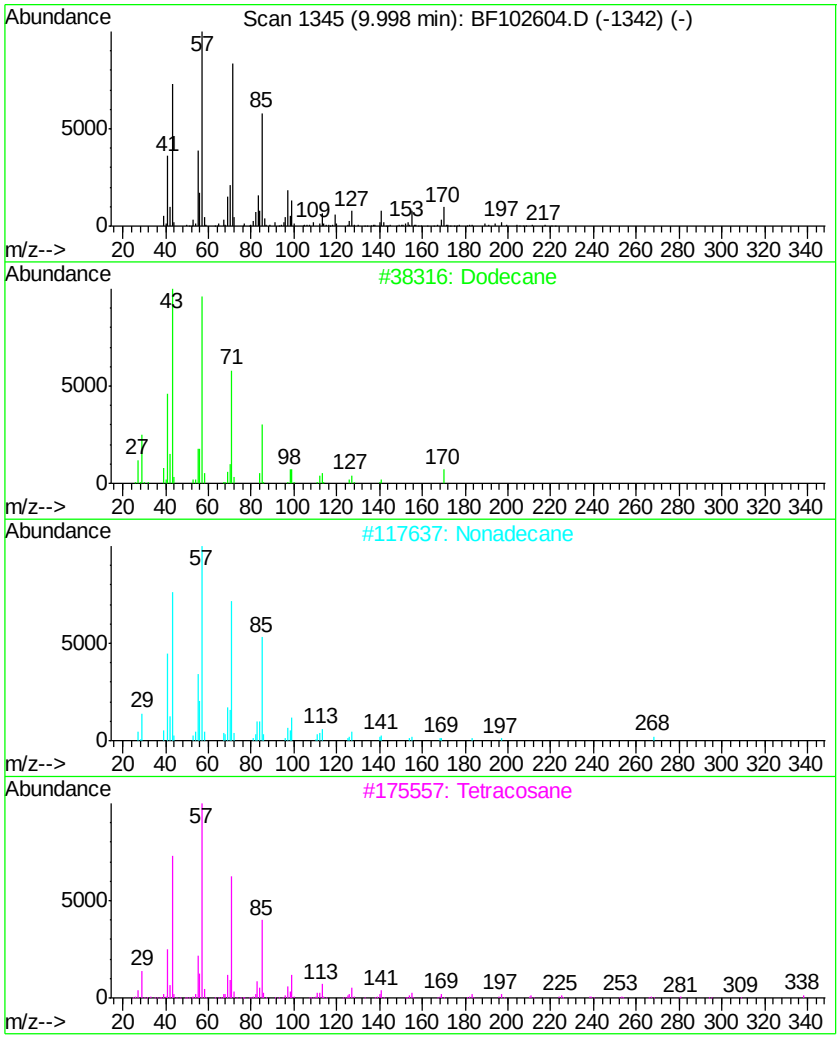
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

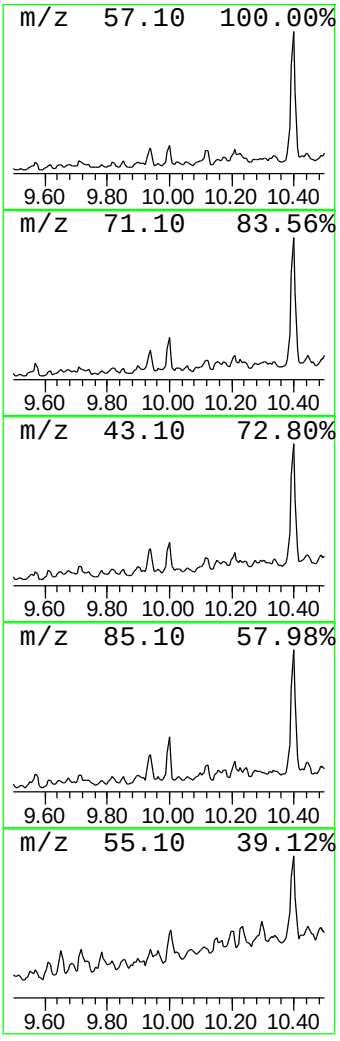
****

Peak Number 8 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.00	6.56 ng	444486	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	74
2	Nonadecane	268	C19H40	000629-92-5	72
3	Tetracosane	338	C24H50	000646-31-1	72
4	Tritetracontane	605	C43H88	007098-21-7	72
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102604.D
Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

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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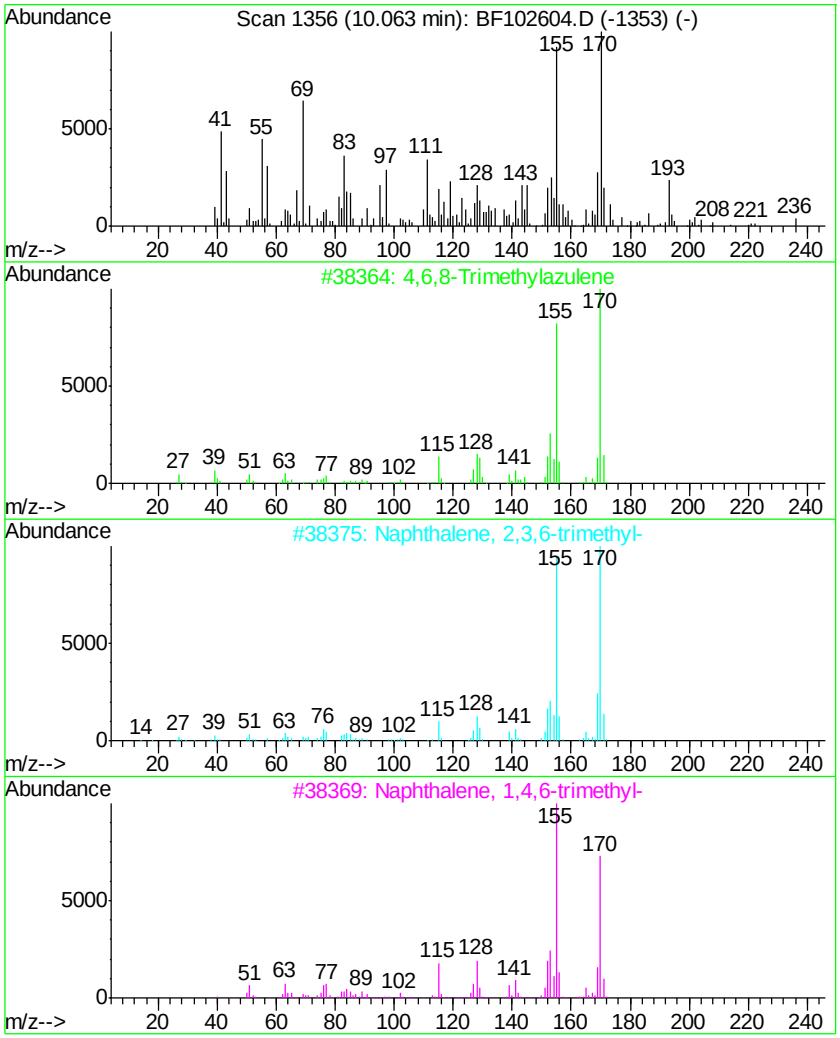
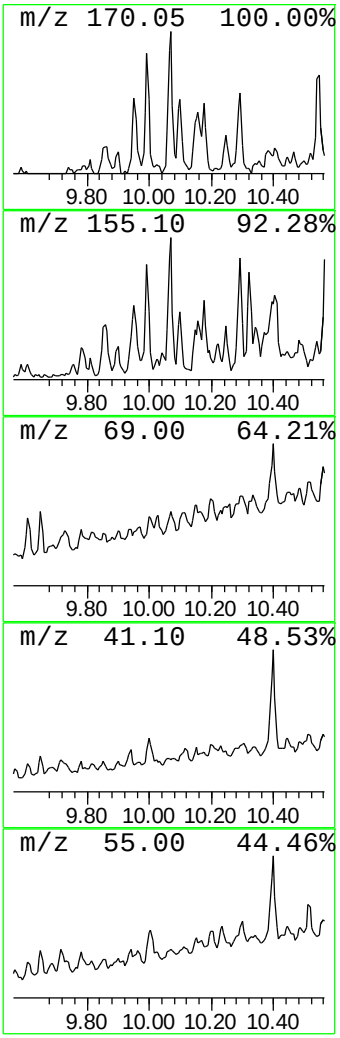
Peak Number 9 4,6,8-Trimethylazulene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.06	4.22 ng	285797	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	96
2	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	95
3	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	95
4	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	93
5	1-(2,2-Dimethylcyclopropyl)-2-ph...	170	C13H14	1000294-91-1	76





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102604.D
Acq On : 29 Jan 2018 18:34
Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

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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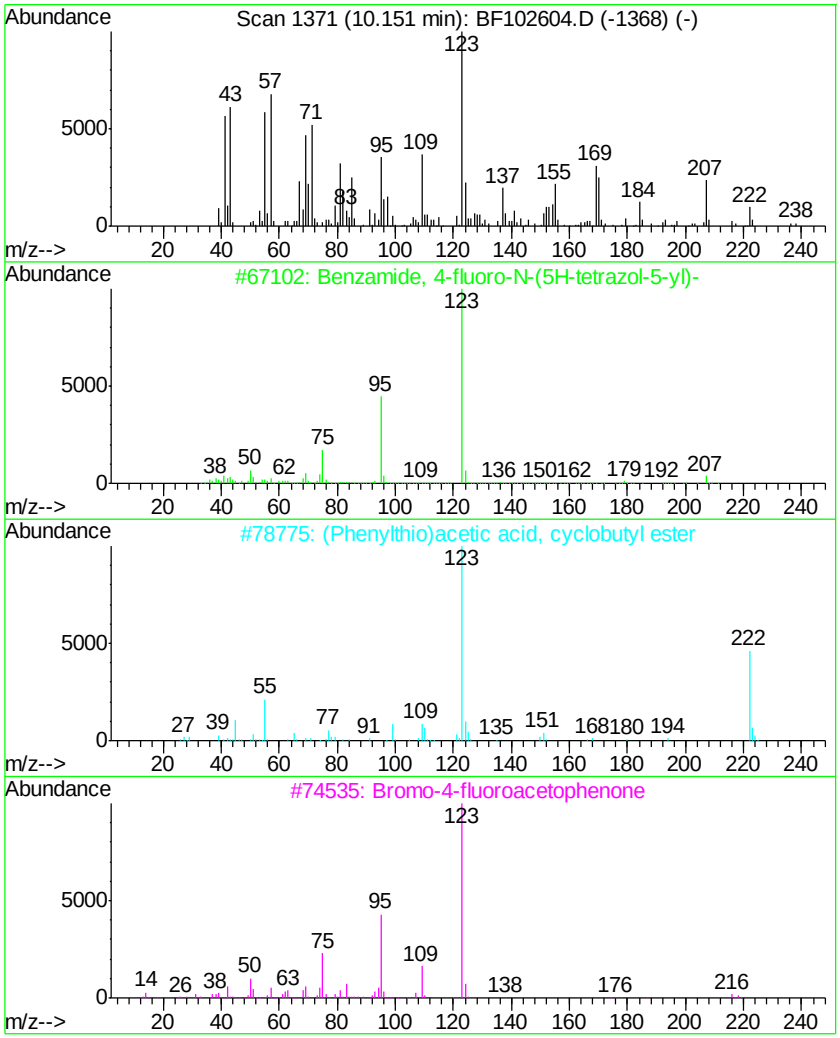
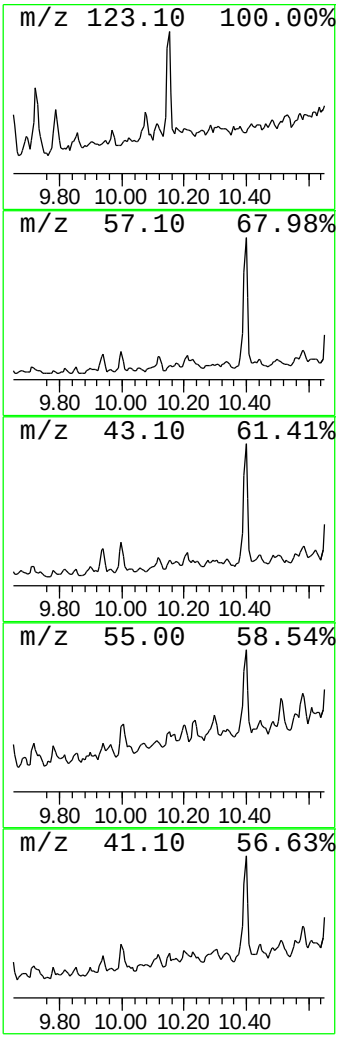
Peak Number 10 unknown10.15 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	4.03 ng	273182	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, 4-fluoro-N-(5H-tetraz...	207	C8H6FN5O	1000262-68-4	30
2	(Phenylthio)acetic acid, cyclobu...	222	C12H14O2S	1000299-95-5	27
3	Bromo-4-fluoroacetophenone	216	C8H6BrFO	000403-29-2	27
4	2-(2-Ethyl-1,3-dimethyl-cyclopen...	182	C12H22O	1000186-82-4	27
5	Methyl 2-fluorobenzoate	154	C8H7FO2	000394-35-4	25





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Data File : BF102604.D
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Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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TIC Integration Parameters: LSCINT.P

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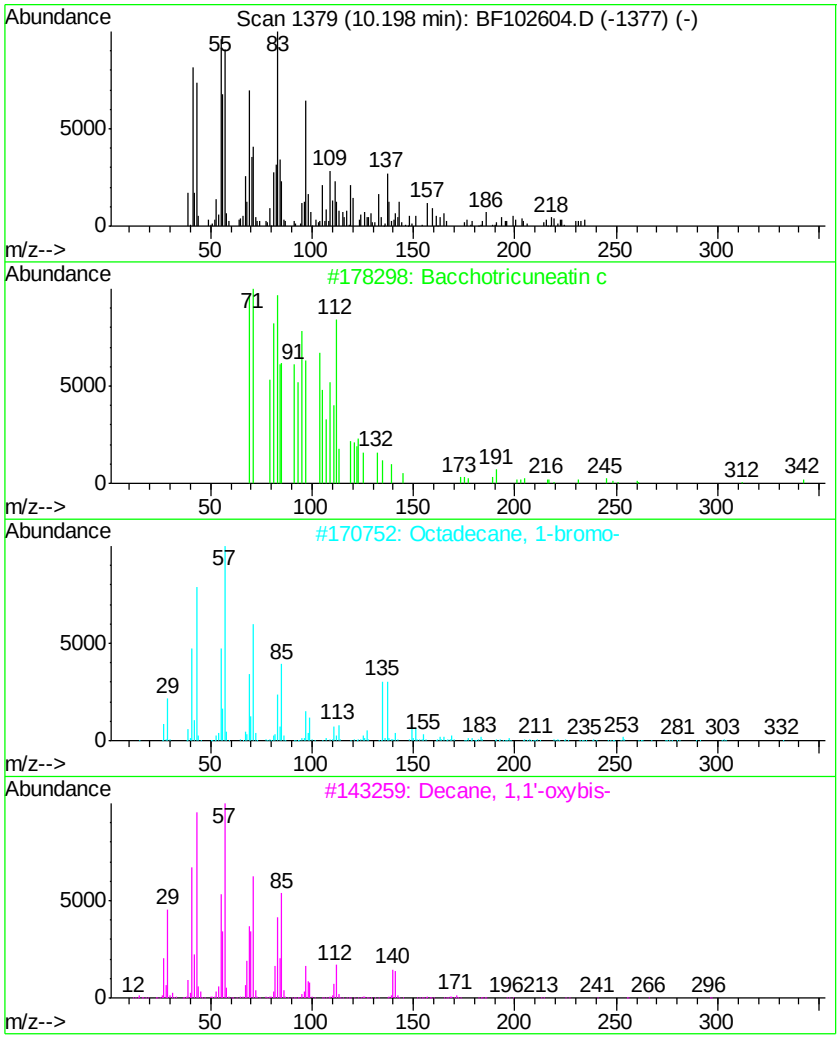
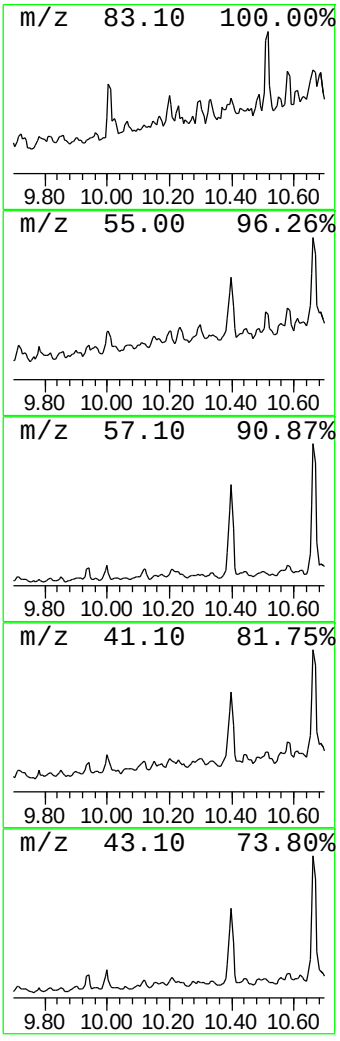
Peak Number 11 Bacchotricuneatin c Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.20	3.31 ng	224195	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	95
2	Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	58
3	Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	52
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	49
5	Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	43





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Data File : BF102604.D
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Operator : SJ/JU
Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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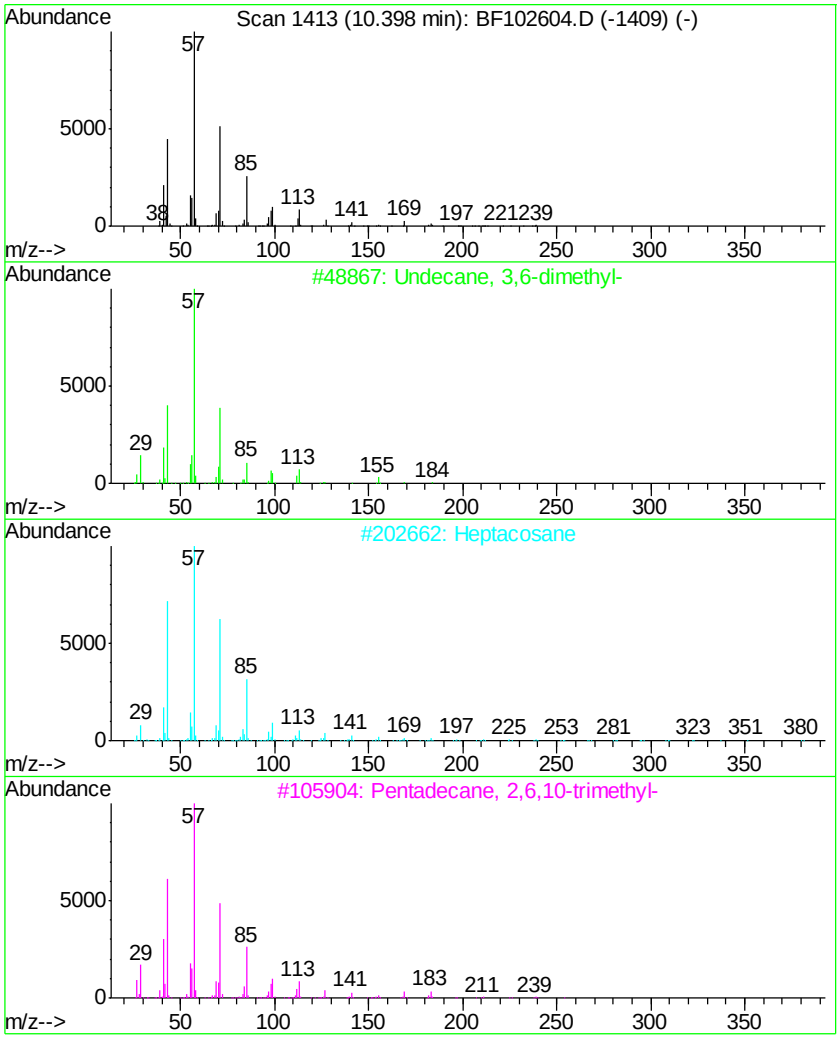
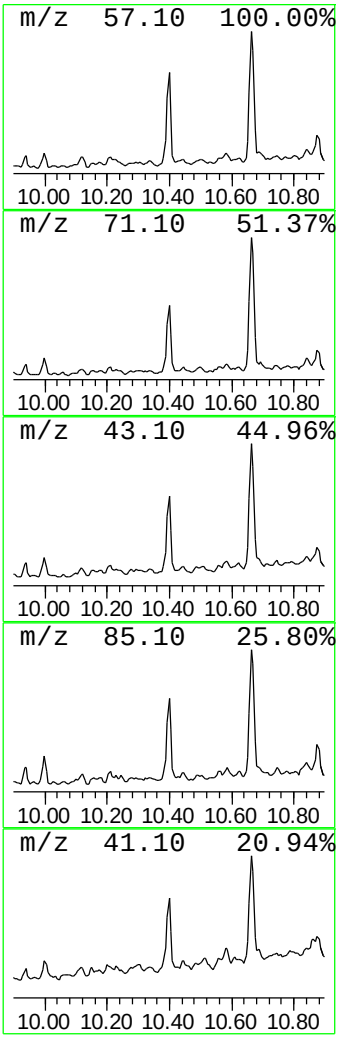
Peak Number 12 Undecane, 3,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	21.02 ng	1424750	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	93
2	Heptacosane	380	C27H56	000593-49-7	90
3	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
4	Hexadecane	226	C16H34	000544-76-3	86
5	Tetracosane	338	C24H50	000646-31-1	80





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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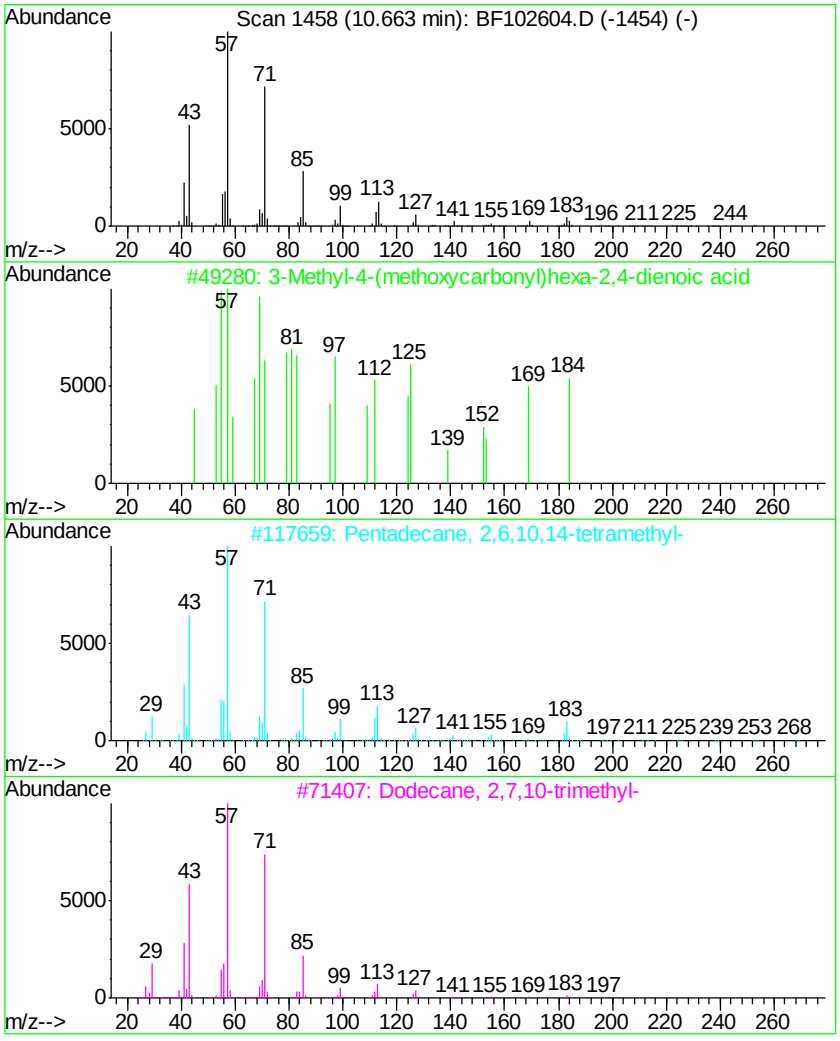
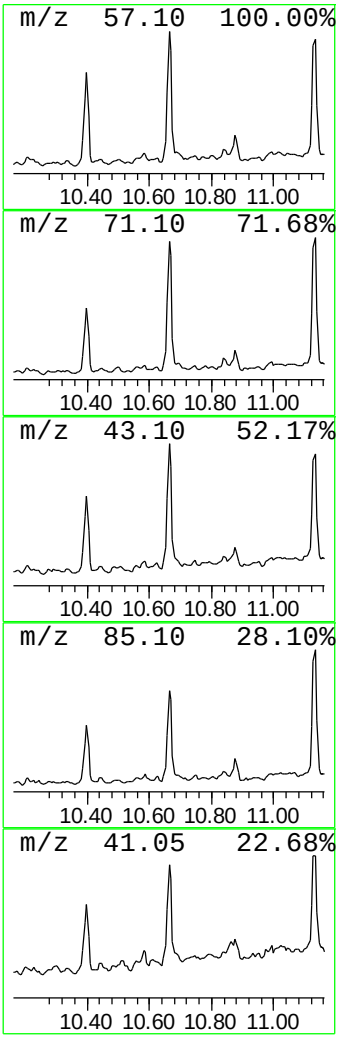
Peak Number 13 3-Methyl-4-(methoxycarbonyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	38.80 ng	2877870	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1000104-10-8	90
2	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4	Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
5	Tridecane	184	C13H28	000629-50-5	72





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Sample : J1257-11 2X
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-16(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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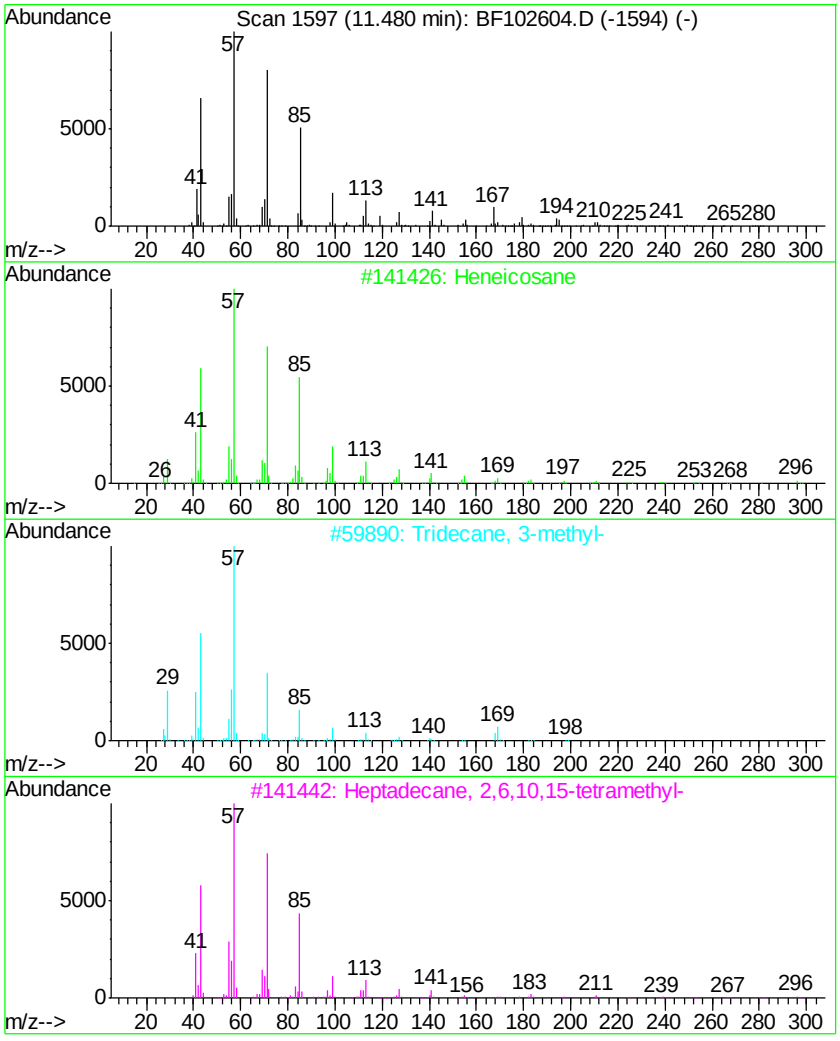
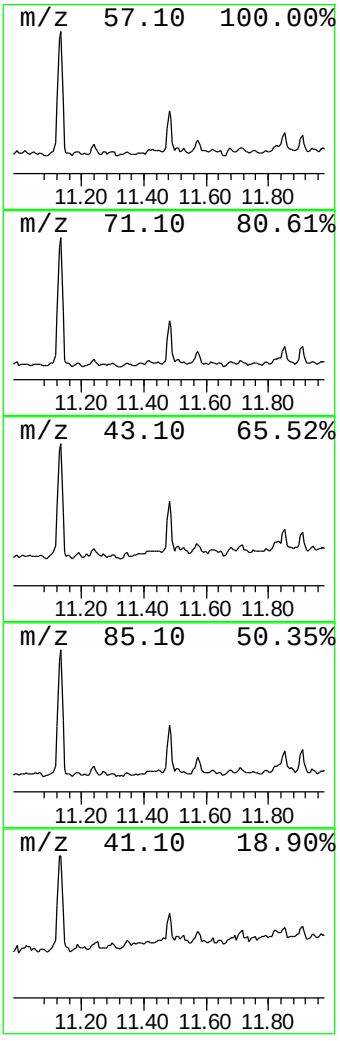
Peak Number 15 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.48	12.02 ng	891605	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	83
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	83
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5	Octadecane	254	C18H38	000593-45-3	80





Tentatively Identified Compound (LSC) summary

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Operator : SJ/JU
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Misc :
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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
unknown6.48	6.48	34.6	ng	1753440	1	6.71	1013380	20.0
Dodecane, 2,6,10-...	9.01	3.3	ng	225582	3	9.75	1355460	20.0
Oxalic acid, ally...	9.15	2.7	ng	183655	3	9.75	1355460	20.0
unknown9.51	9.61	4.6	ng	308718	3	9.75	1355460	20.0
unknown9.65	9.65	3.2	ng	214447	3	9.75	1355460	20.0
Tridecane	9.94	3.5	ng	240321	3	9.75	1355460	20.0
Dodecane	10.00	6.6	ng	444486	3	9.75	1355460	20.0
4,6,8-Trimethylaz...	10.06	4.2	ng	285797	3	9.75	1355460	20.0
unknown10.15	10.15	4.0	ng	273182	3	9.75	1355460	20.0
Bacchotricuneatin c	10.20	3.3	ng	224195	3	9.75	1355460	20.0
Undecane, 3,6-dim...	10.40	21.0	ng	1424750	3	9.75	1355460	20.0
3-Methyl-4-(metho...	10.66	38.8	ng	2877870	4	11.24	1483550	20.0
Heneicosane	11.48	12.0	ng	891605	4	11.24	1483550	20.0