LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098569.D
Acq On : 15 Sep 2017 15:06
Operator : SJ/JU
Sample : I5188-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

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-BF091117.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	3.528	236	245	258	rBV	635303	1077748	37.14%	3.696%
2	4.816	461	464	476	rBV	215960	297576	10.26%	1.020%
3	5.198	524	529	534	rBV2	32611	48917	1.69%	0.168%
4	5.251	534	538	553	rVV	2657110	2735486	94.28%	9.381%
5	6.304	713	717	727	rBV	2587734	2901568	100.00%	9.950%
6	6.416	732	736	742	rVV	3228271	2880372	99.27%	9.878%
7	6.475	742	746	751	rVB2	90336	124192	4.28%	0.426%
8	6.640	771	774	781	rVB	931611	901502	31.07%	3.092%
9	6.798	797	801	808	rBV	2489624	2122006	73.13%	7.277%
10	7.216	867	872	875	rBV	1748110	1720052	59.28%	5.899%
11	7.245	875	877	882	rVB	111612	92758	3.20%	0.318%
12	7.657	943	947	950	rBV4	22777	37641	1.30%	0.129%
13	7.698	950	954	957	rVB2	36146	41810	1.44%	0.143%
14	7.928	988	993	995	rBV	1386048	1236076	42.60%	4.239%
15	7.951	995	997	1002	rVB	377925	344773	11.88%	1.182%
16	8.351	1062	1065	1070	rBV2	26534	38521	1.33%	0.132%
17	8.522	1091	1094	1097	rBV	94005	80214	2.76%	0.275%
18	8.639	1111	1114	1118	rBV	219584	162820	5.61%	0.558%
19	8.739	1127	1131	1134	rBV	129100	112182	3.87%	0.385%
20	8.810	1139	1143	1146	rBV6	25208	40681	1.40%	0.140%
21	8.857	1149	1151	1158	rBV5	36536	63162	2.18%	0.217%
22	8.951	1164	1167	1171	rVB3	37886	43943	1.51%	0.151%
23	9.004	1171	1176	1179	rBV	3168216	2700616	93.07%	9.261%
24	9.086	1185	1190	1192	rBV	103130	121293	4.18%	0.416%
25	9.198	1207	1209	1213	rBV	26776	31137	1.07%	0.107%
26	9.263	1217	1220	1224	rBV2	61516	91073	3.14%	0.312%
27	9.339	1230	1233	1236	rBV	80368	80369	2.77%	0.276%
28	9.369	1236	1238	1241	rVV2	53192	55500	1.91%	0.190%
29	9.404	1241	1244	1247	rVB	386692	321797	11.09%	1.104%
30	9.457	1251	1253	1257	rVB2	39680	42449	1.46%	0.146%
31	9.539	1264	1267	1270	rBV	126014	110445	3.81%	0.379%
32	9.616	1277	1280	1283	rBV	125251	105095	3.62%	0.360%
33	9.681	1287	1291	1294	rVV	1281154	1166517	40.20%	4.000%
34	9.710	1294	1296	1301	rVB4	37423	51718	1.78%	0.177%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098569.D
Acq On : 15 Sep 2017 15:06
Operator : SJ/JU
Sample : I5188-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.881	1322	1325	1327	rBV2	52109	61230	2.11%	0.210%
36	9.904	1327	1329	1331	rVB2	79432	60407	2.08%	0.207%
37	9.998	1342	1345	1347	rBV3	37558	49043	1.69%	0.168%
38	10.081	1356	1359	1361	rBV3	48307	51542	1.78%	0.177%
39	10.116	1362	1365	1370	rVB2	99101	103188	3.56%	0.354%
40	10.222	1381	1383	1386	rBV2	50281	53287	1.84%	0.183%
41	10.333	1400	1402	1407	rVB2	56208	54155	1.87%	0.186%
42	10.469	1421	1425	1429	rBV	1351592	1195656	41.21%	4.100%
43	10.586	1442	1445	1454	rVB2	204778	303338	10.45%	1.040%
44	11.033	1519	1521	1523	rBV	107467	89771	3.09%	0.308%
45	11.063	1524	1526	1530	rVB2	104617	104123	3.59%	0.357%
46	11.163	1539	1543	1545	rBV	1175844	977890	33.70%	3.354%
47	11.186	1545	1547	1550	rVB	321086	257548	8.88%	0.883%
48	12.374	1746	1749	1751	rVB	301296	239308	8.25%	0.821%
49	12.598	1785	1787	1790	rBV	239290	214077	7.38%	0.734%
50	12.745	1809	1812	1816	rBV	1736610	1676174	57.77%	5.748%
51	13.804	1988	1992	1994	rBV	846473	875160	30.16%	3.001%
52	15.210	2227	2231	2237	rVB	647056	812240	27.99%	2.785%

Sum of corrected areas: 29160146

LSC Report - Integrated Chromatogram

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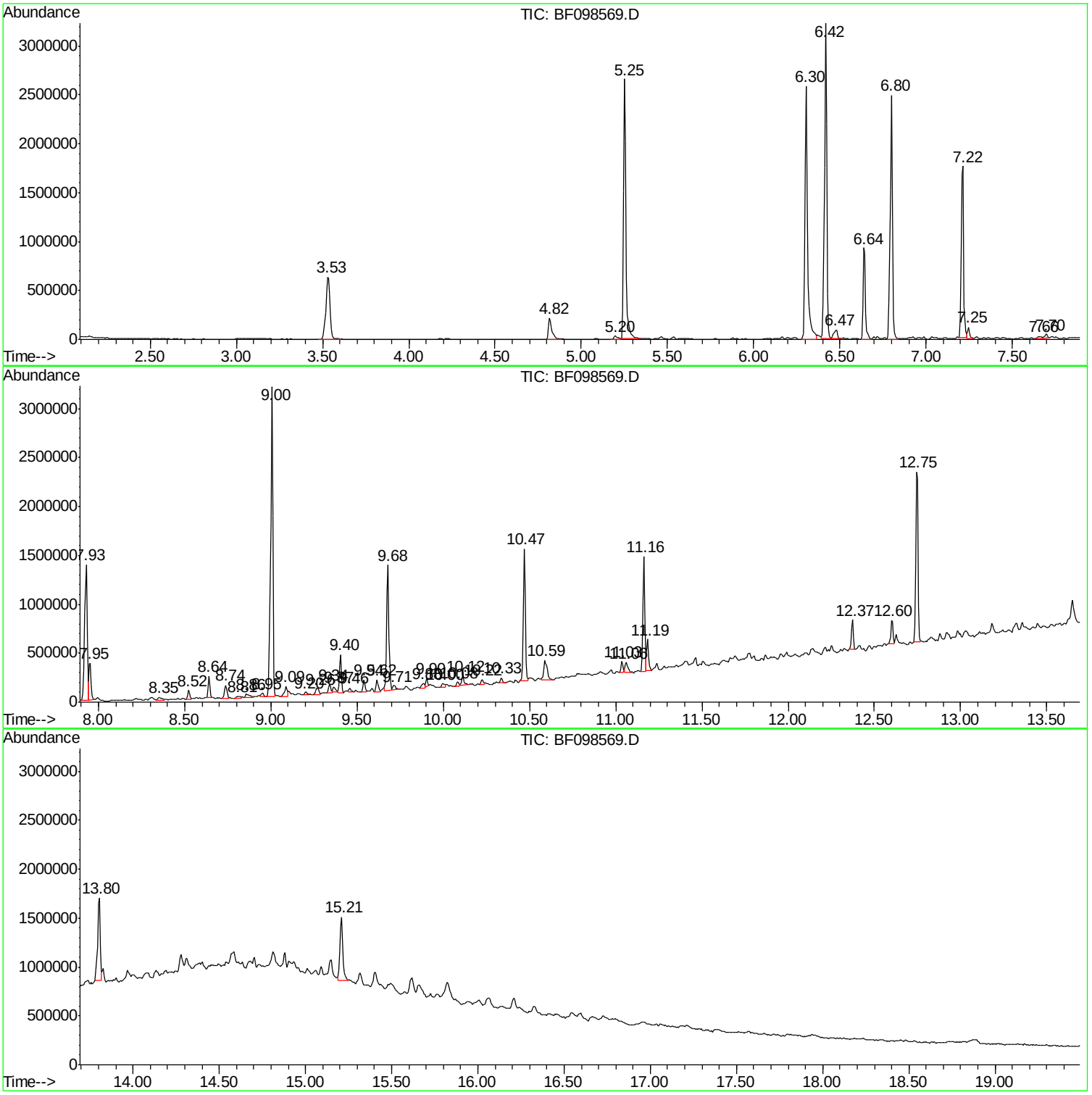
Acq On : 15 Sep 2017 15:06
Operator : SJ/JU
Sample : I5188-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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\BF091517\
Data File : BF098569.D
Acq On : 15 Sep 2017 15:06
Operator : SJ/JU
Sample : I5188-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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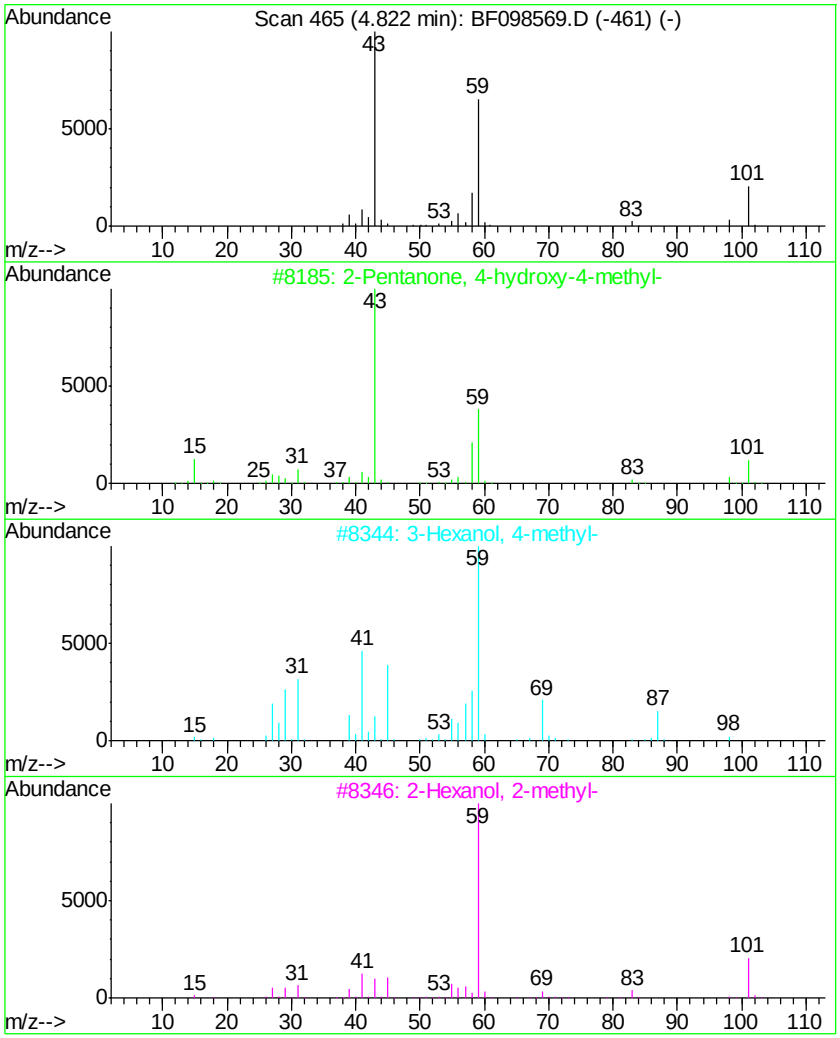
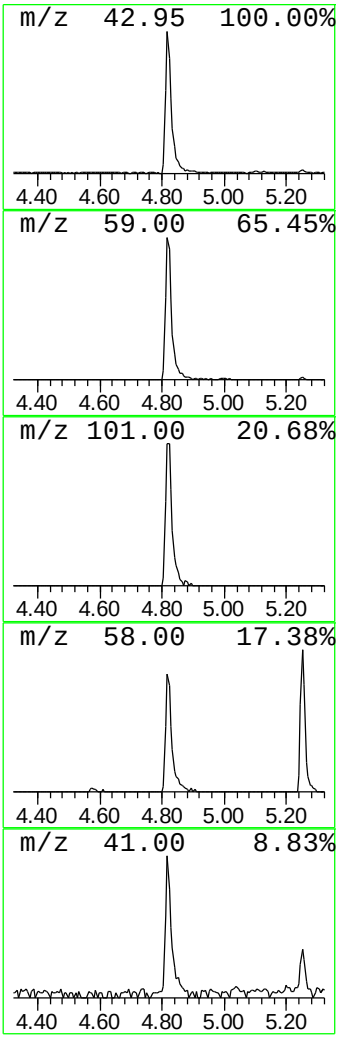
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	6.60 ng	297576	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098569.D
Acq On : 15 Sep 2017 15:06
Operator : SJ/JU
Sample : I5188-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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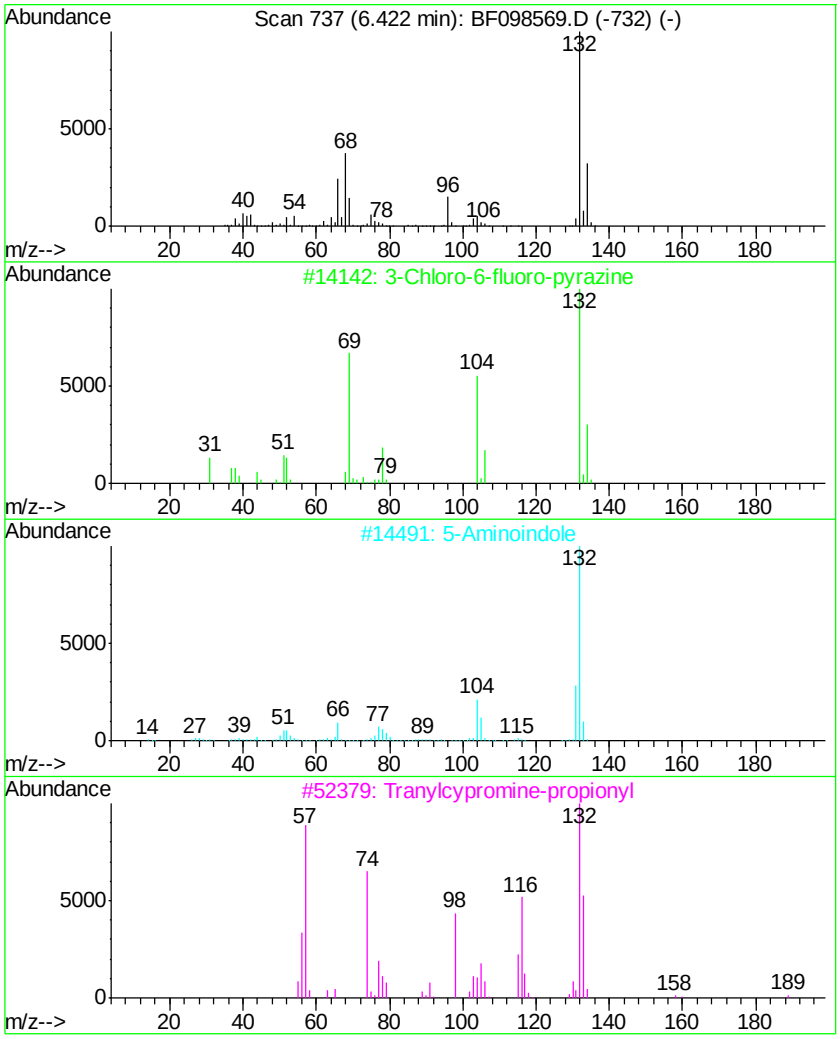
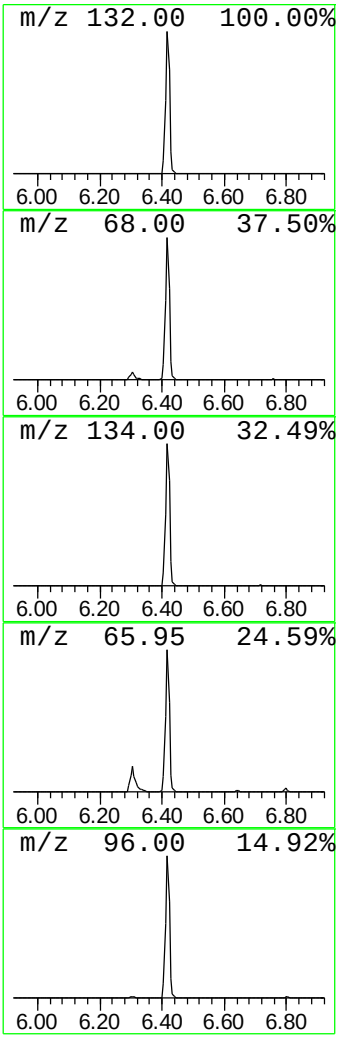
Peak Number 3 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	63.90 ng	2880370	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098569.D
Acq On : 15 Sep 2017 15:06
Operator : SJ/JU
Sample : I5188-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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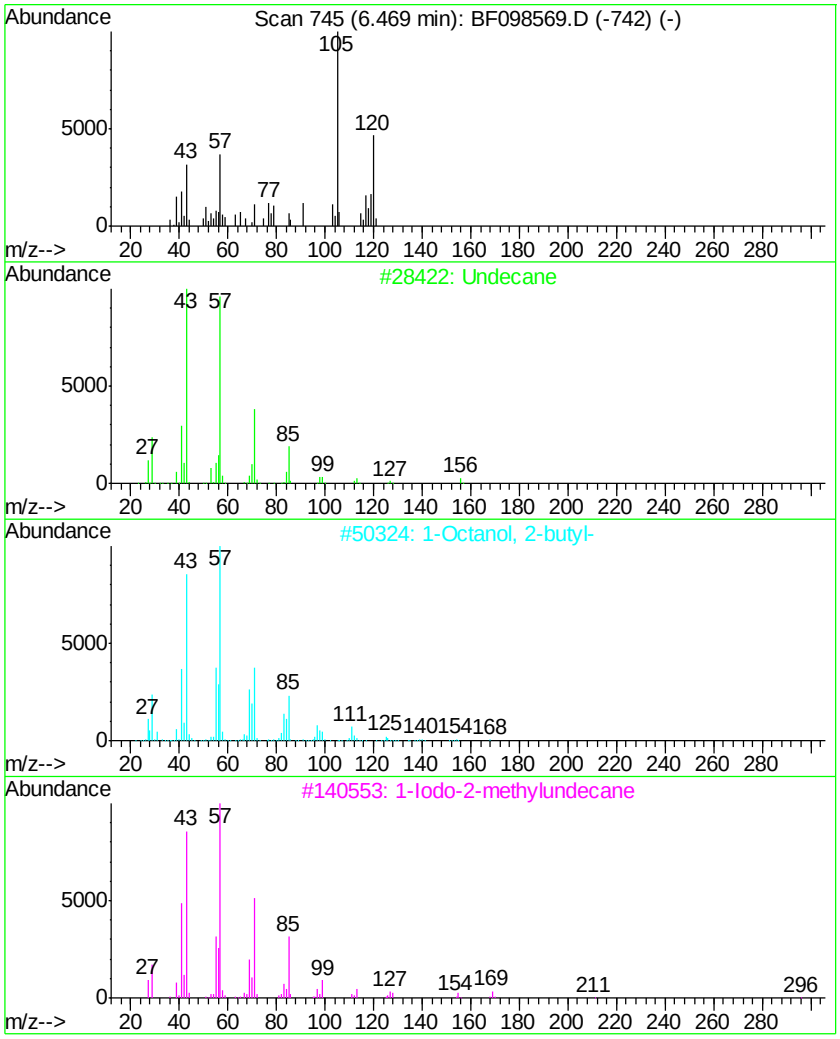
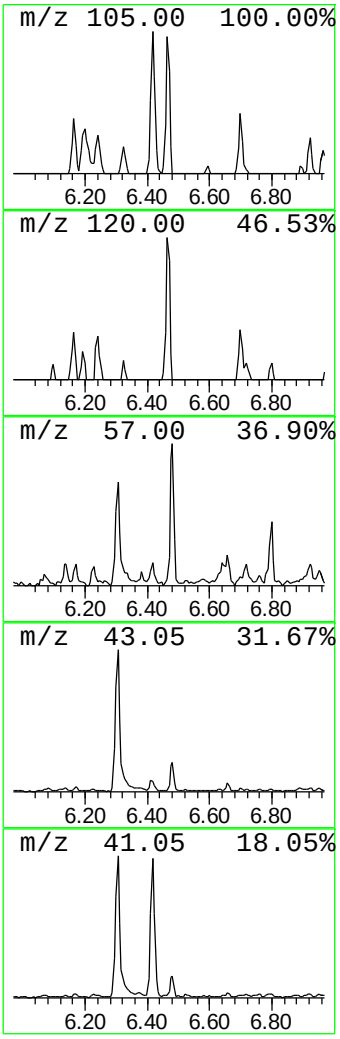
Peak Number 4 Undecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	2.76 ng	124192	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	50
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	50
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	47
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	47
5	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
Data File : BF098569.D
Acq On : 15 Sep 2017 15:06
Operator : SJ/JU
Sample : I5188-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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TIC Integration Parameters: LSCINT.P

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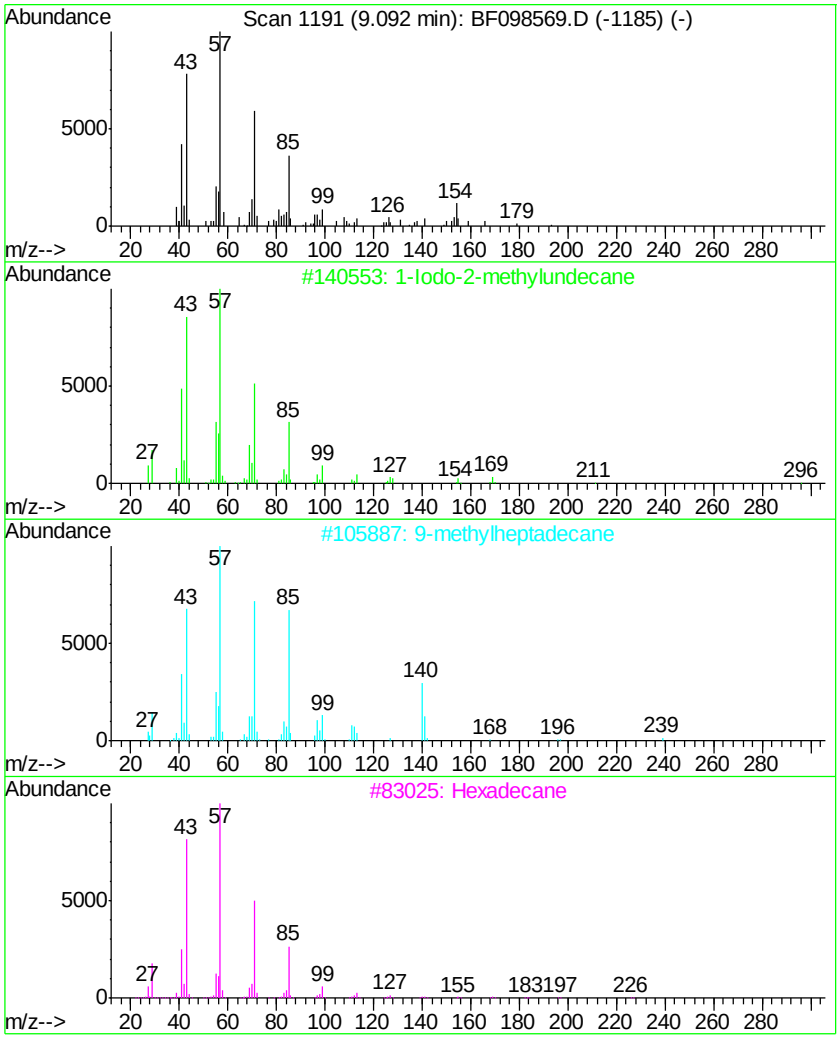
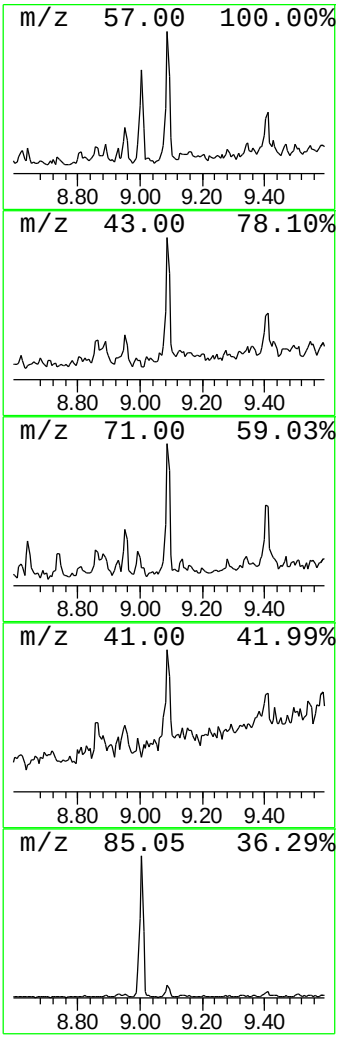
Peak Number 6 1-Iodo-2-methylundecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	2.08 ng	121293	Acenaphthene-d10	9.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80
2	9-methylheptadecane	254	C18H38	026741-18-4	64
3	Hexadecane	226	C16H34	000544-76-3	59
4	Nonane, 5-(1-methylpropyl)-	184	C13H28	062185-54-0	59
5	Tetradecane	198	C14H30	000629-59-4	59





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Acq On : 15 Sep 2017 15:06
Operator : SJ/JU
Sample : I5188-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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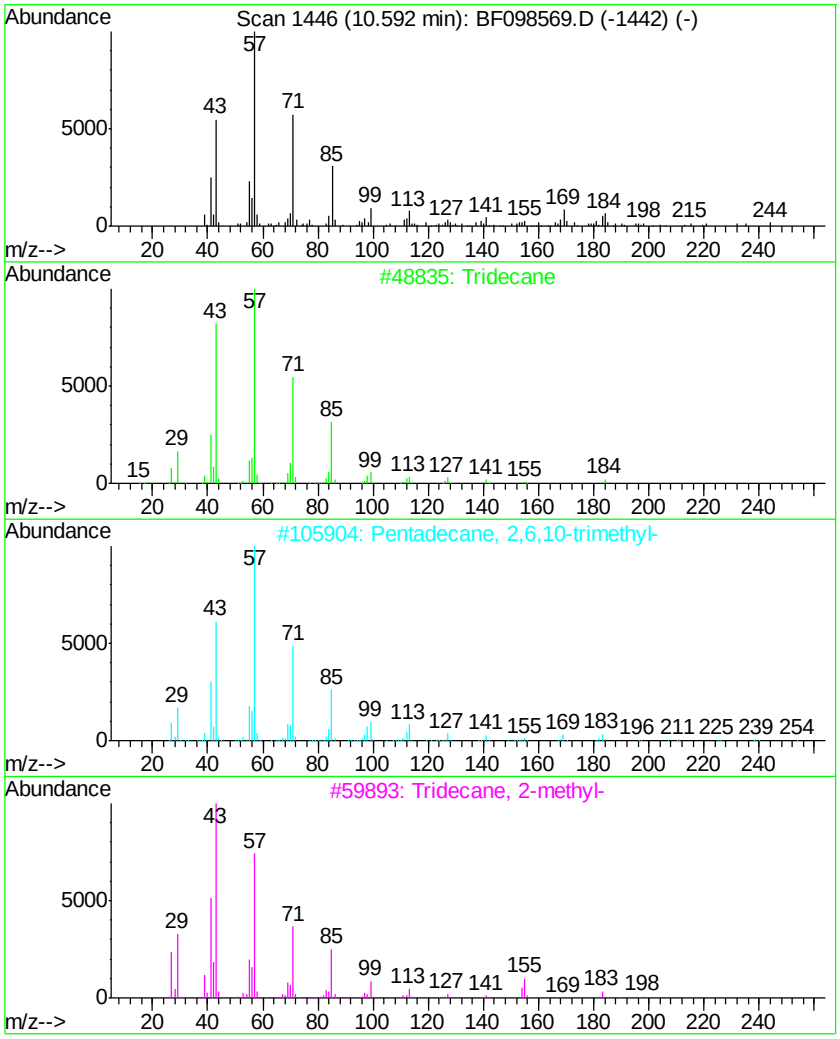
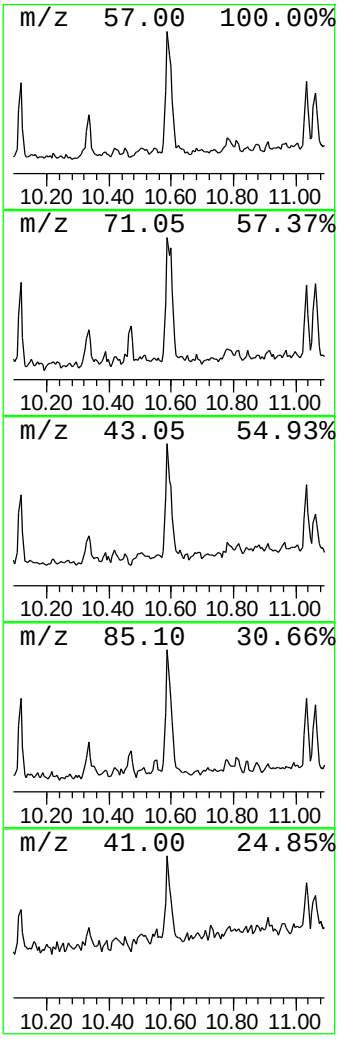
Peak Number 7 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	6.20 ng	303338	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	96
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
4	Undecane, 2-methyl-	170	C12H26	007045-71-8	80
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	72





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Acq On : 15 Sep 2017 15:06
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Sample : I5188-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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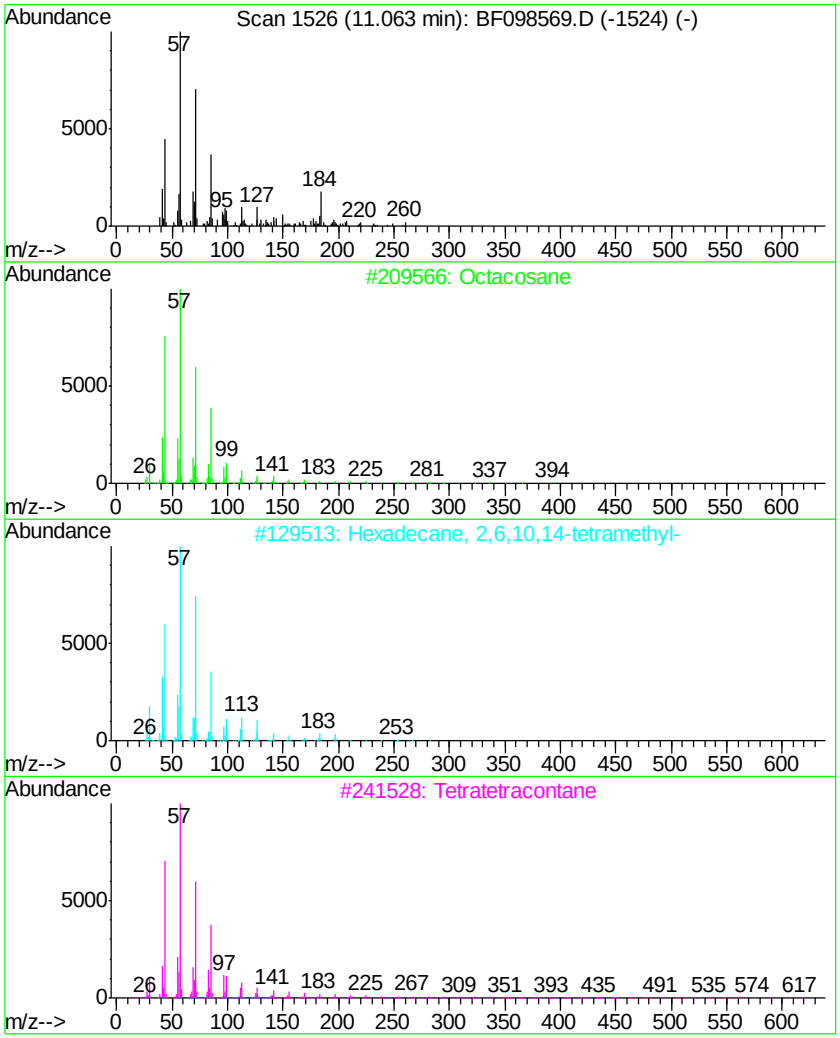
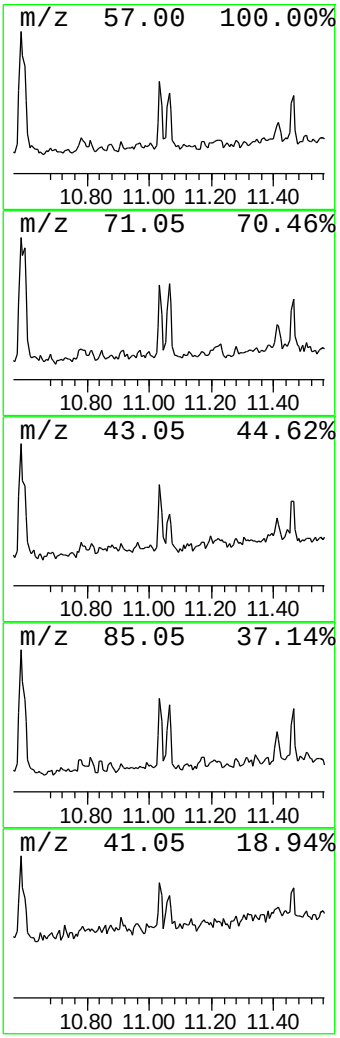
Peak Number 8 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	2.13 ng	104123	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	72
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
3	Tetratetracontane	619	C44H90	007098-22-8	72
4	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	68
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091517\
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Acq On : 15 Sep 2017 15:06
Operator : SJ/JU
Sample : I5188-07
Misc :
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Instrument : BNA_F
ClientSampleId : RL-4-12.25-24.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.82	6.6	ng	297576	1	6.64	901502	20.0
unknown6.42	6.42	63.9	ng	2880370	1	6.64	901502	20.0
Undecane	6.47	2.8	ng	124192	1	6.64	901502	20.0
1-Iodo-2-methylun...	9.09	2.1	ng	121293	3	9.68	1166520	20.0
Tridecane	10.59	6.2	ng	303338	4	11.16	977890	20.0
Octacosane	11.06	2.1	ng	104123	4	11.16	977890	20.0