LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

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-BF012417.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	3.196	92	97	99	rBV	33936	71087	1.04%	0.073%
2	3.344	107	110	116	rVB	38933	81088	1.19%	0.083%
3	3.664	135	138	143	rVB	44282	79333	1.16%	0.081%
4	3.858	152	155	161	rBV	41563	69875	1.02%	0.072%
5	4.441	203	206	211	rVB3	59279	119889	1.75%	0.123%
6	4.533	211	214	216	rBV	56053	71936	1.05%	0.074%
7	4.944	247	250	253	rBV	76901	86036	1.26%	0.088%
8	5.059	256	260	263	rVV3	33050	81214	1.19%	0.083%
9	5.150	266	268	272	rVV	655895	762249	11.14%	0.781%
10	5.230	272	275	278	rVV3	90029	215229	3.15%	0.221%
11	5.276	278	279	282	rVV	130822	139849	2.04%	0.143%
12	5.356	284	286	289	rVV	64146	87472	1.28%	0.090%
13	5.481	295	297	300	rBV	188258	191703	2.80%	0.196%
14	5.573	302	305	307	rBV	2121174	2378412	34.76%	2.437%
15	5.687	312	315	318	rBV4	59094	126600	1.85%	0.130%
16	5.744	318	320	323	rVB	135368	198668	2.90%	0.204%
17	5.801	323	325	326	rBV	67643	85991	1.26%	0.088%
18	5.847	326	329	330	rVV3	154974	170894	2.50%	0.175%
19	6.007	337	343	345	rBV3	248531	430647	6.29%	0.441%
20	6.122	352	353	355	rBV	63355	75981	1.11%	0.078%
21	6.179	355	358	360	rBV3	104917	257841	3.77%	0.264%
22	6.213	360	361	364	rVB2	79073	125293	1.83%	0.128%
23	6.270	364	366	371	rVB2	256468	414728	6.06%	0.425%
24	6.362	371	374	375	rBV3	86314	154564	2.26%	0.158%
25	6.396	375	377	378	rBV2	88569	129748	1.90%	0.133%
26	6.430	378	380	381	rVB	159760	178553	2.61%	0.183%
27	6.476	381	384	388	rBV3	180575	480692	7.03%	0.493%
28	6.567	390	392	393	rBV	130999	132336	1.93%	0.136%
29	6.602	393	395	399	rVB	1286983	1753872	25.63%	1.797%
30	6.693	399	403	404	rBV2	75826	116028	1.70%	0.119%
31	6.739	404	407	409	rBV	3642592	3802237	55.57%	3.896%
32	6.773	409	410	412	rVV2	320931	428206	6.26%	0.439%
33	6.819	412	414	415	rVB2	282216	374515	5.47%	0.384%
34	6.899	419	421	425	rBV2	442173	700090	10.23%	0.717%

LSC Area Percent Report

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Operator : SJ/MA
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Misc :
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Instrument : BNA_F
ClientSampleId : MW-03

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 >
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	6.967	425	427	429	rBV	1236786	1350126	19.73%	1.383%
36	7.013	429	431	432	rVB	115699	150228	2.20%	0.154%
37	7.036	432	433	436	rVB	351893	328996	4.81%	0.337%
38	7.127	438	441	443	rBV	3525502	3748807	54.79%	3.841%
39	7.162	443	444	446	rBV	199675	291740	4.26%	0.299%
40	7.242	450	451	454	rVB3	68326	104026	1.52%	0.107%
41	7.299	454	456	461	rVB4	219517	498477	7.28%	0.511%
42	7.367	461	462	464	rBV2	277338	469979	6.87%	0.482%
43	7.413	464	466	470	rVB2	391141	768822	11.24%	0.788%
44	7.482	470	472	475	rBV3	332282	883900	12.92%	0.906%
45	7.539	475	477	481	rVV	2446589	3508209	51.27%	3.595%
46	7.607	481	483	486	rVB4	308272	707251	10.34%	0.725%
47	7.665	486	488	492	rBV4	293300	601988	8.80%	0.617%
48	7.779	497	498	501	rBV3	257346	389977	5.70%	0.400%
49	7.836	501	503	505	rBV3	199079	321966	4.71%	0.330%
50	7.905	507	509	510	rBV2	219443	318266	4.65%	0.326%
51	7.939	510	512	515	rVB2	607490	948442	13.86%	0.972%
52	7.996	515	517	520	rBV3	482280	1069723	15.63%	1.096%
53	8.076	520	524	527	rBV5	791512	1650304	24.12%	1.691%
54	8.202	534	535	537	rVB2	258989	248549	3.63%	0.255%
55	8.270	537	541	543	rBV2	1622173	2963165	43.30%	3.036%
56	8.316	543	545	549	rVB3	610964	1292096	18.88%	1.324%
57	8.373	549	550	553	rVB3	388644	447672	6.54%	0.459%
58	8.442	553	556	558	rBV4	868753	1747741	25.54%	1.791%
59	8.499	558	561	562	rBV	1936333	2815744	41.15%	2.885%
60	8.602	569	570	572	rBV2	457059	487322	7.12%	0.499%
61	8.636	572	573	576	rVB3	371251	505217	7.38%	0.518%
62	8.693	576	578	579	rBV2	992895	1298447	18.98%	1.330%
63	8.750	580	583	586	rVB4	756219	1705411	24.92%	1.747%
64	8.796	586	587	589	rVB2	432880	493578	7.21%	0.506%
65	8.842	589	591	592	rVB2	382468	449674	6.57%	0.461%
66	8.876	592	594	596	rBV2	300800	534971	7.82%	0.548%
67	8.933	597	599	601	rVB3	539492	652173	9.53%	0.668%
68	8.990	601	604	606	rBV4	680357	1562174	22.83%	1.601%
69	9.036	606	608	609	rBV	705973	933657	13.64%	0.957%
70	9.082	610	612	613	rVV2	921263	897926	13.12%	0.920%
71	9.116	613	615	616	rVB2	310870	402047	5.88%	0.412%

LSC Area Percent Report

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Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

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
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	9.230	623	625	627	rBV2	482202	880713	12.87%	0.902%
73	9.356	634	636	637	rVB	3535865	3515216	51.37%	3.602%
74	9.390	637	639	642	rVB3	1030517	1572024	22.97%	1.611%
75	9.550	652	653	655	rVB2	642983	575921	8.42%	0.590%
76	9.722	664	668	670	rBV4	840222	2465619	36.03%	2.526%
77	9.939	685	687	689	rBV3	725843	1159809	16.95%	1.188%
78	10.030	693	695	697	rVV2	786485	1137657	16.63%	1.166%
79	10.271	714	716	720	rVB4	775578	1658143	24.23%	1.699%
80	10.476	729	734	740	rBV2	1938931	6842555	100.00%	7.011%
81	10.579	741	743	745	rVB3	820352	1246135	18.21%	1.277%
82	10.762	757	759	763	rVB2	804484	1351726	19.75%	1.385%
83	10.842	763	766	769	rVB	1670443	2539262	37.11%	2.602%
84	10.945	773	775	780	rVV4	1374552	3069191	44.85%	3.145%
85	11.048	780	784	786	rVV4	878338	2417560	35.33%	2.477%
86	11.093	786	788	792	rVB4	1069571	2175049	31.79%	2.229%
87	11.242	800	801	804	rVV	767359	669031	9.78%	0.686%
88	11.288	804	805	809	rVB	849654	1150834	16.82%	1.179%
89	11.425	815	817	819	rVB2	973838	1469861	21.48%	1.506%
90	11.528	824	826	829	rVB	1229152	1631406	23.84%	1.672%
91	12.088	873	875	885	rVB3	774801	1341315	19.60%	1.374%
92	12.316	892	895	897	rBV	374131	539630	7.89%	0.553%
93	12.854	940	942	945	rVB	227884	241215	3.53%	0.247%
94	13.117	962	965	968	rVB	3241978	3646081	53.29%	3.736%
95	13.997	1040	1042	1051	rVB	128328	276346	4.04%	0.283%
96	14.168	1054	1057	1059	rVB	1017260	1010437	14.77%	1.035%
97	15.642	1183	1186	1191	rVB	607891	889257	13.00%	0.911%

Sum of corrected areas: 97593640

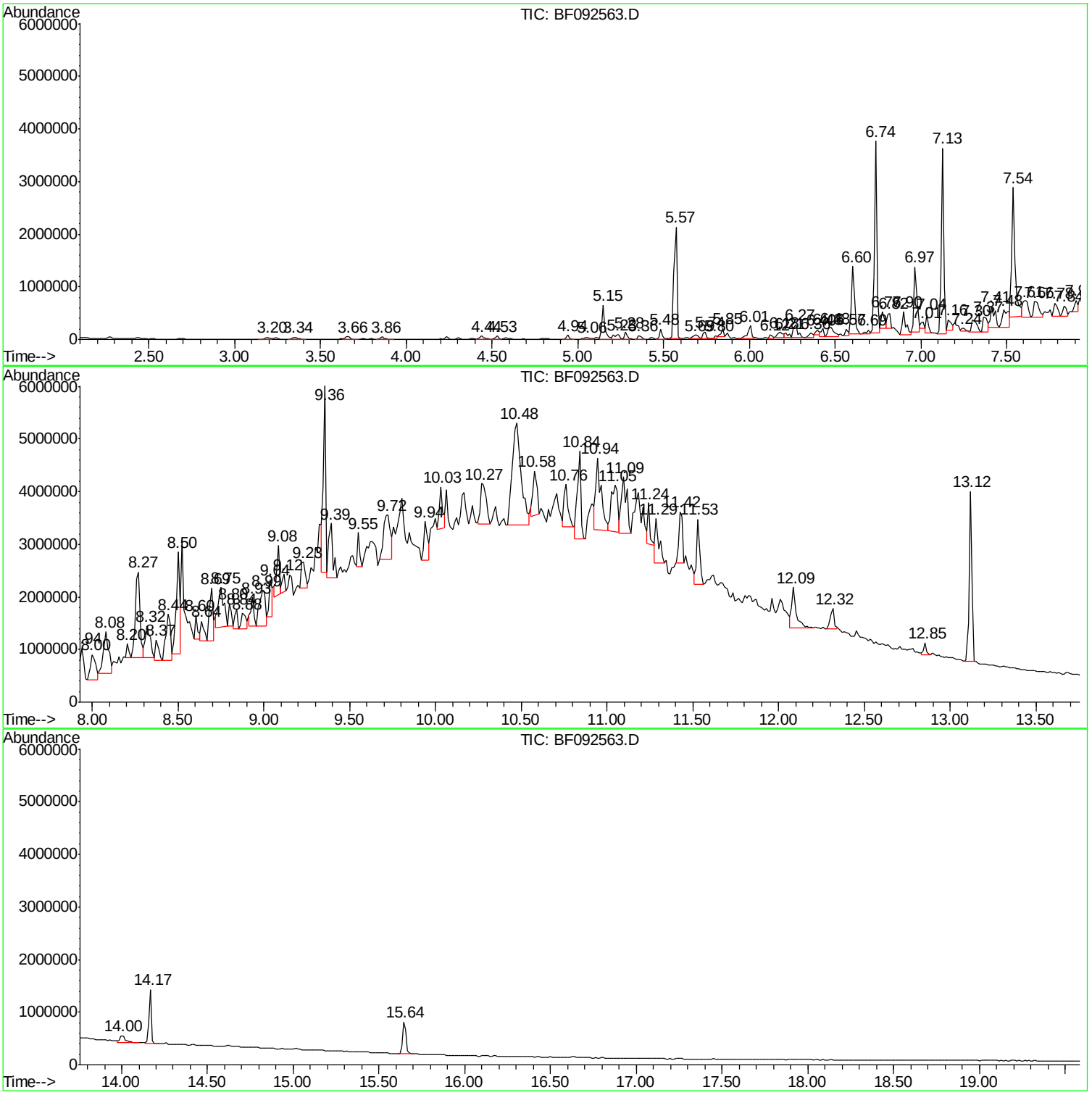
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

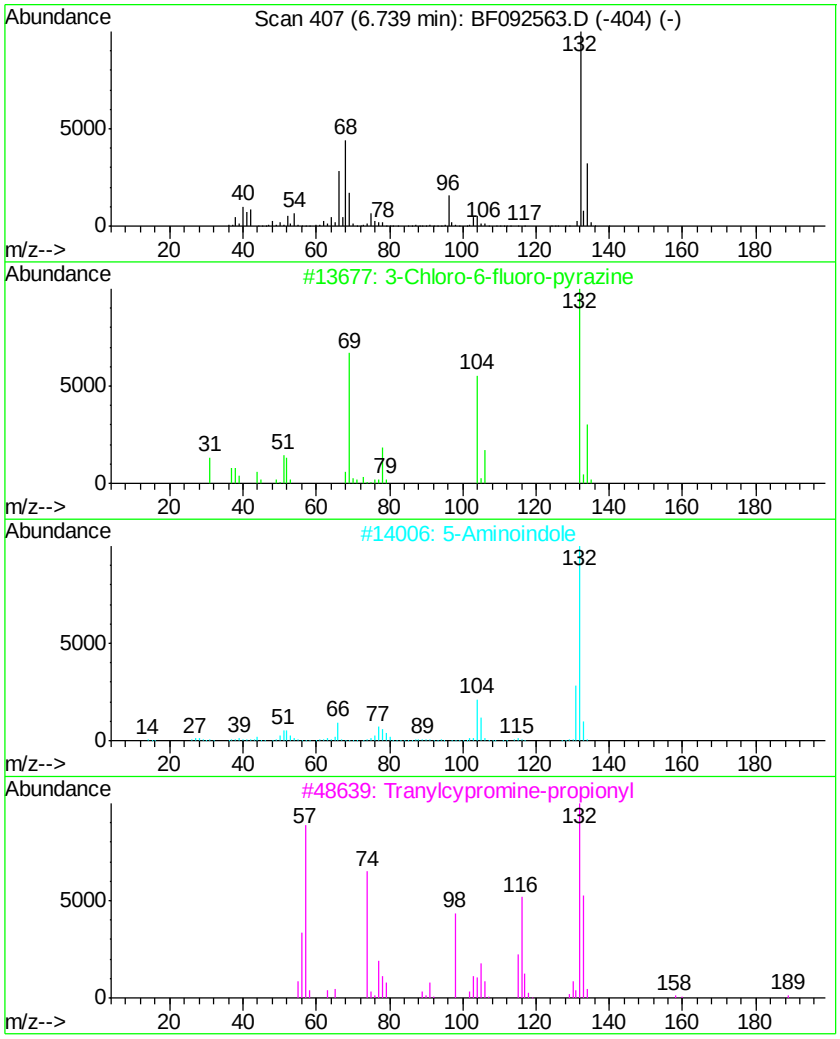
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

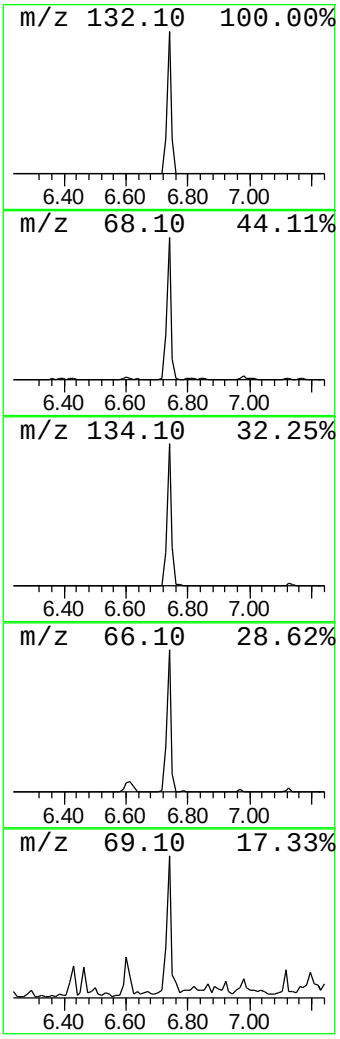
****

Peak Number 1 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	56.32 ng	3802240	1,4-Dichlorobenzene-d4	6.97

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	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

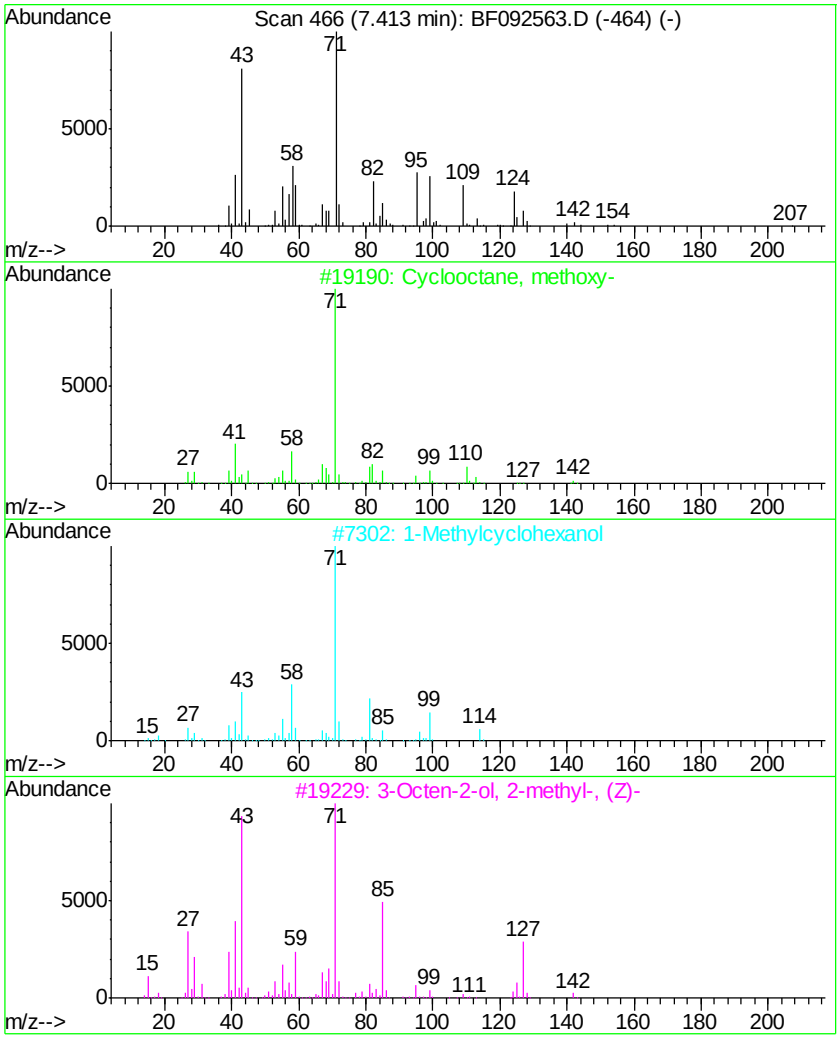
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

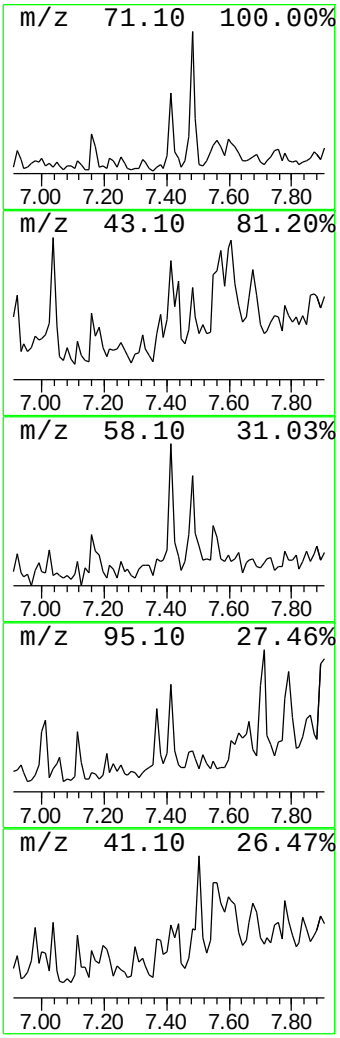
****

Peak Number 3 unknown7.41 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	11.39 ng	768822	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, methoxy-	142	C9H18O	013213-32-6	43
2	1-Methylcyclohexanol	114	C7H14O	000590-67-0	43
3	3-Octen-2-ol, 2-methyl-, (Z)-	142	C9H18O	018521-07-8	38
4	Hexanal, 4,4-dimethyl-	128	C8H16O	005932-91-2	37
5	Silane, ethenyldiethylmethyl-	128	C7H16Si	018292-29-0	35





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

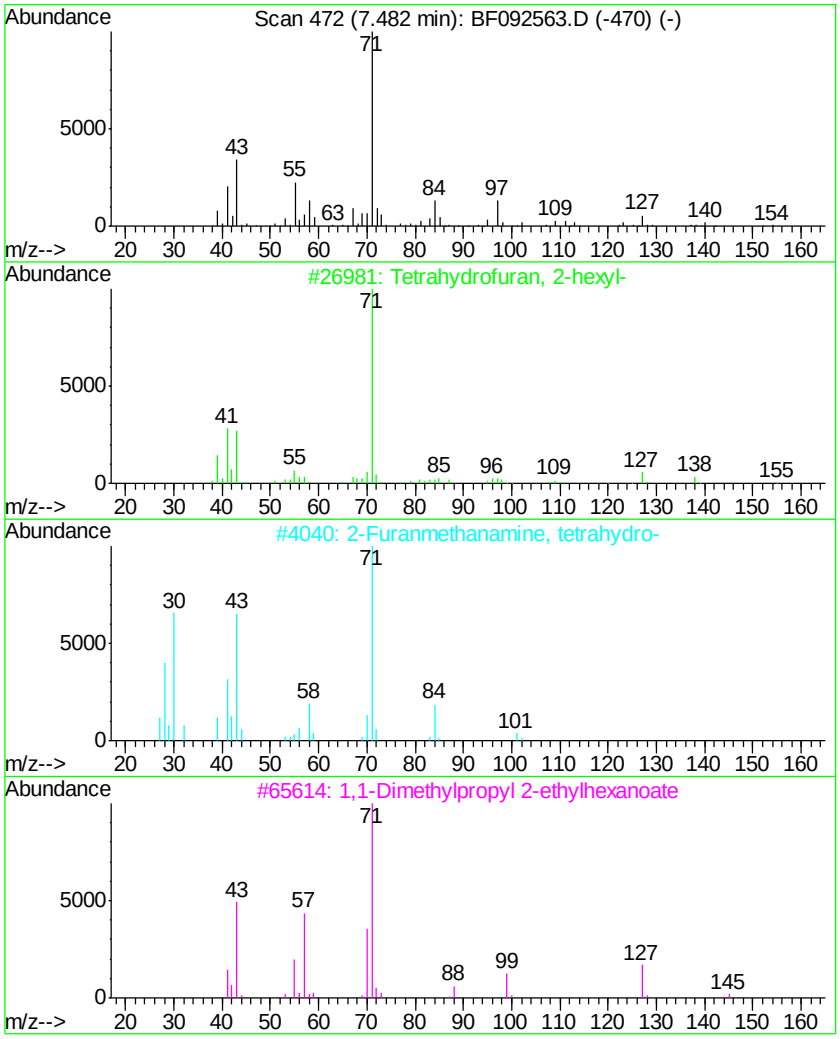
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

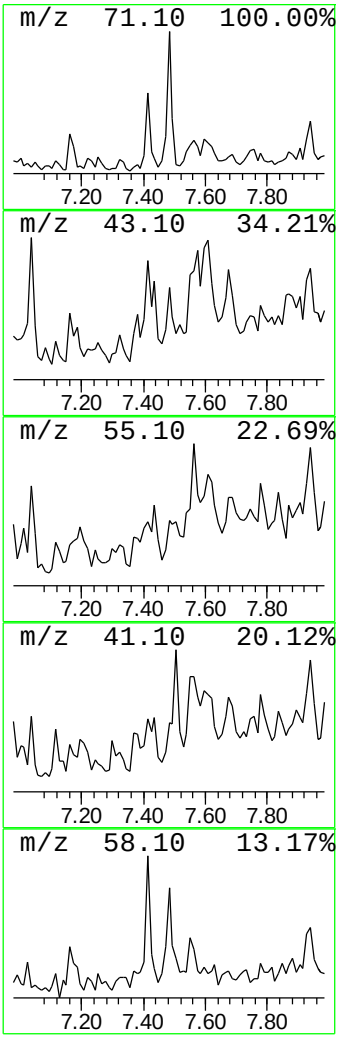
****

Peak Number 4 Tetrahydrofuran, 2-hexyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	13.09 ng	883900	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrahydrofuran, 2-hexyl-	156	C10H20O	003208-32-0	59
2	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	53
3	1,1-Dimethylpropyl 2-ethylhexanoate	214	C13H26O2	1000099-99-2	50
4	3-Cyclopentylpropionic acid, 2-t...	226	C13H22O3	1000293-46-9	50
5	Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

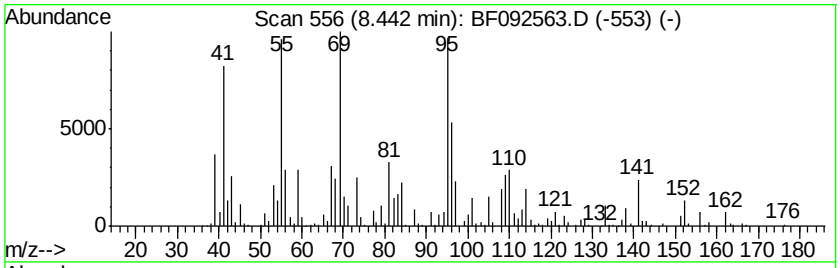
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

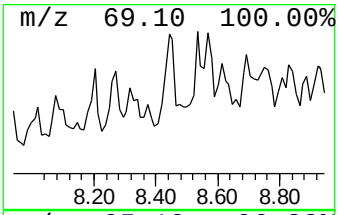
****

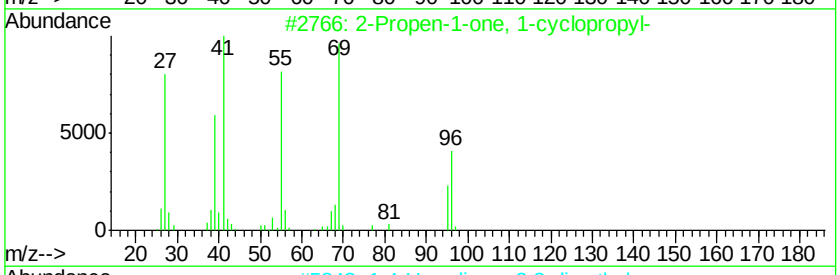
Peak Number 5 unknown8.44 Concentration Rank 18

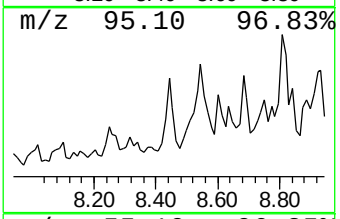
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.44	11.80 ng	1747740	Naphthalene-d8	8.27

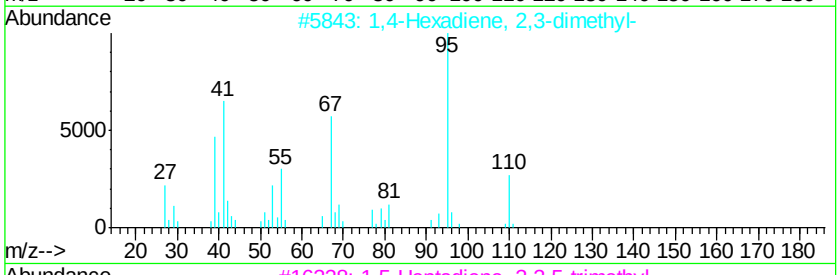
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propen-1-one, 1-cyclopropyl-	96	C6H8O	059819-62-4	30
2	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	25
3	1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	22
4	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	18
5	2-Propenoic acid, 2-methyl-, eth...	114	C6H10O2	000097-63-2	18

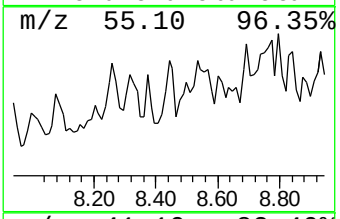


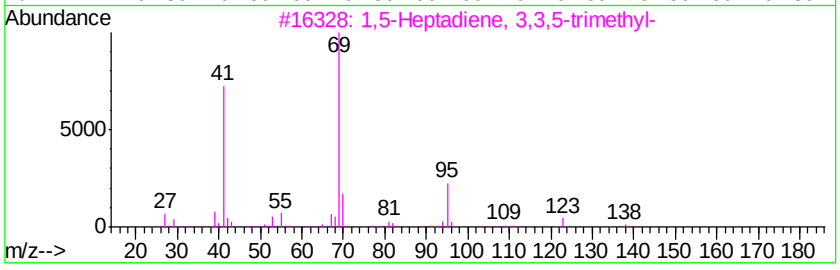


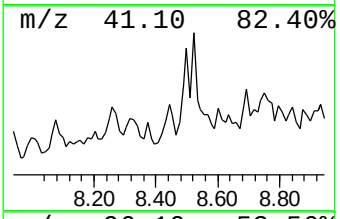


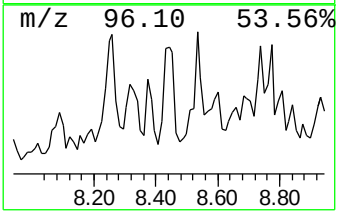












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Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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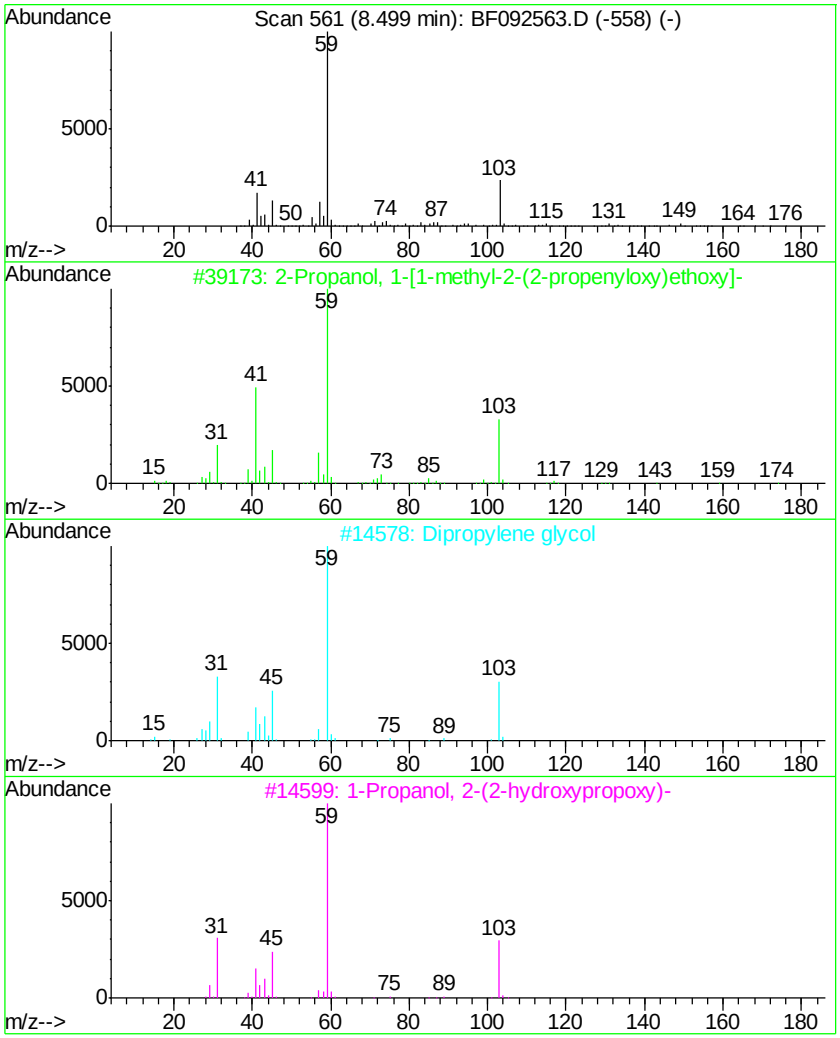
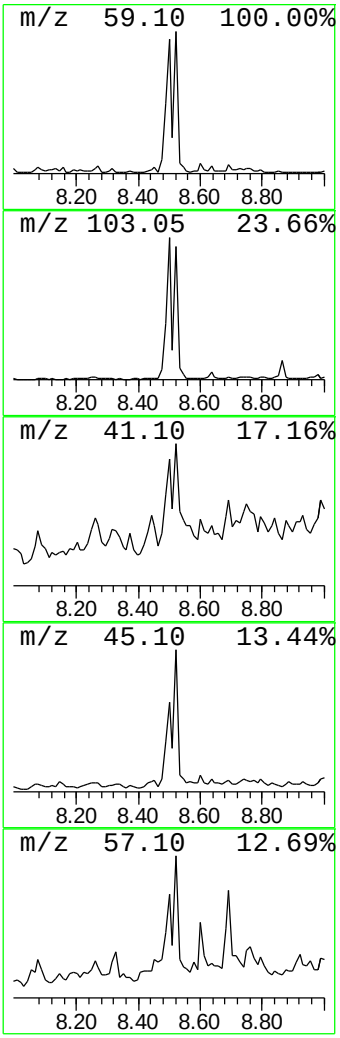
Peak Number 6 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.50	19.01 ng	2815740	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	78
2	Dipropylene glycol	134	C6H14O3	025265-71-8	78
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	72
5	2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	72





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Sample : I1353-01
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ClientSampleId : MW-03

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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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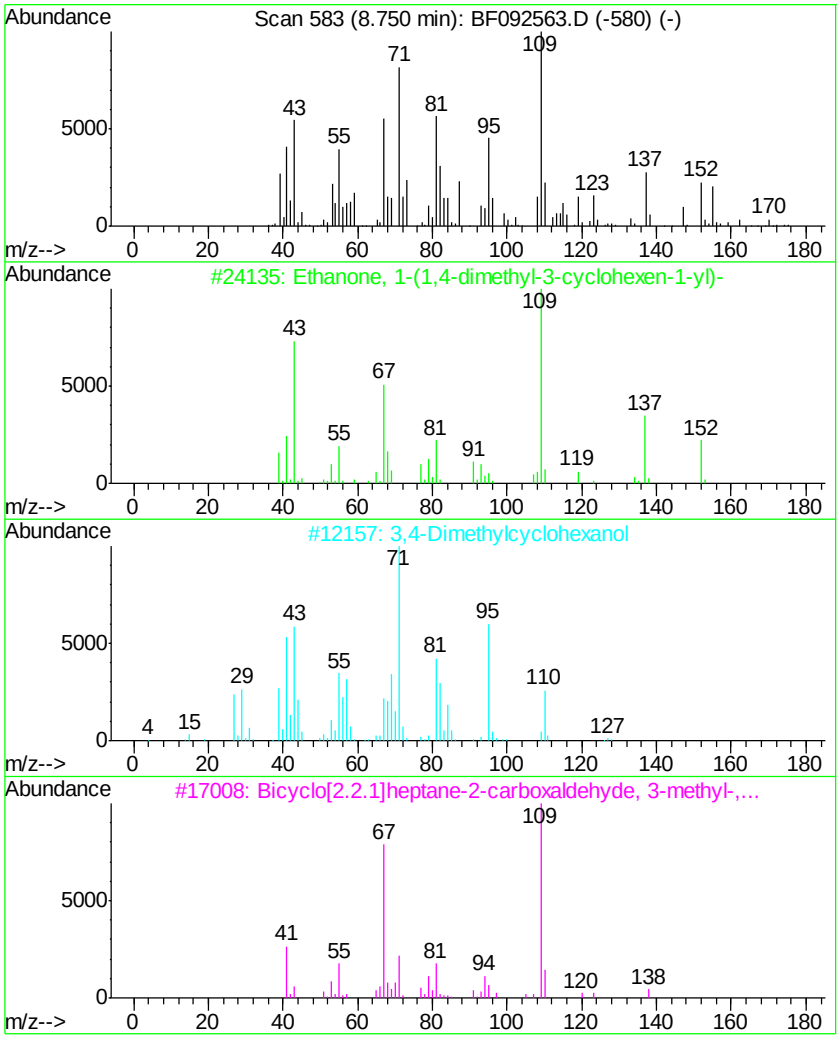
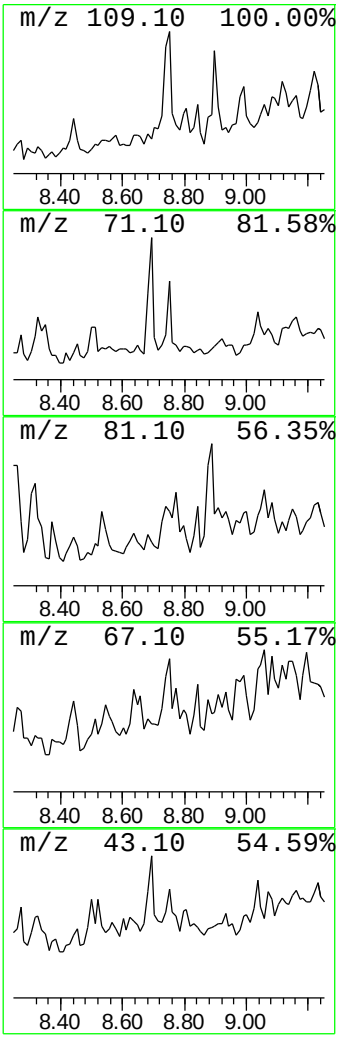
Peak Number 7 unknown8.75 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.75	11.51 ng	1705410	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	38
2	3,4-Dimethylcyclohexanol	128	C8H16O	005715-23-1	30
3	Bicyclo[2.2.1]heptane-2-carboxal...	138	C9H14O	015780-36-6	30
4	Cyclohexanol, 3,5-dimethyl-	128	C8H16O	005441-52-1	30
5	3-Octyne, 7-methyl-	124	C9H16	037050-06-9	30





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Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

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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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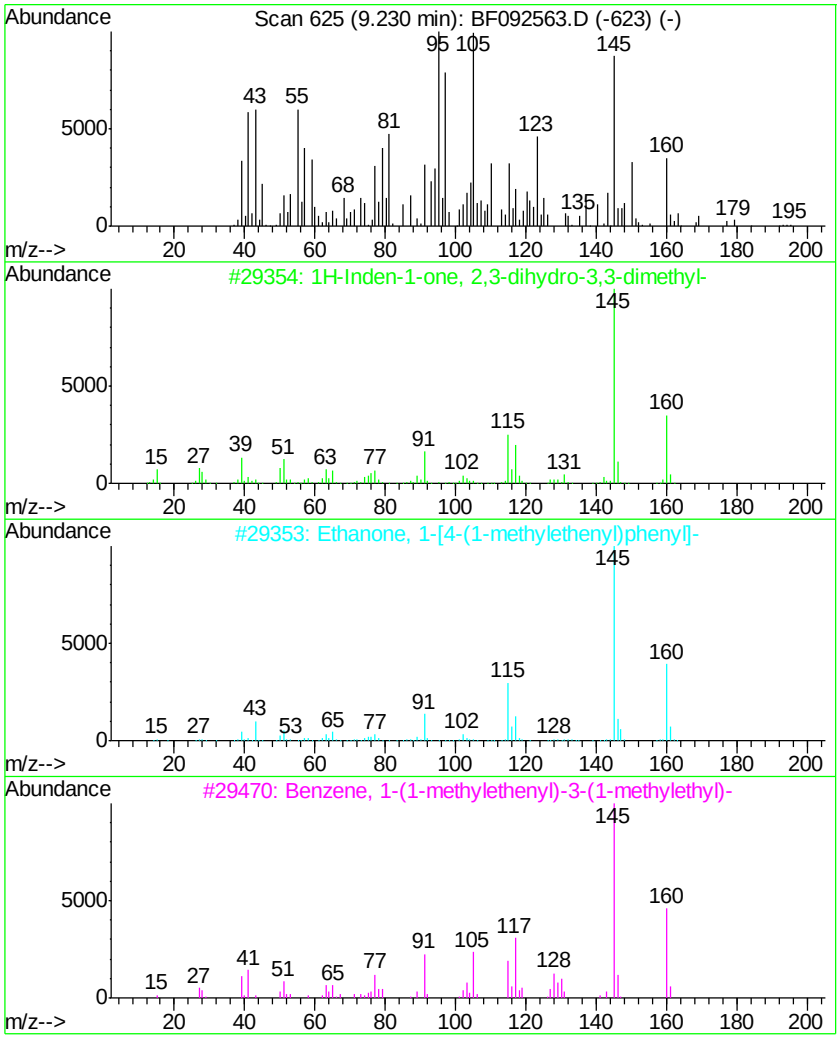
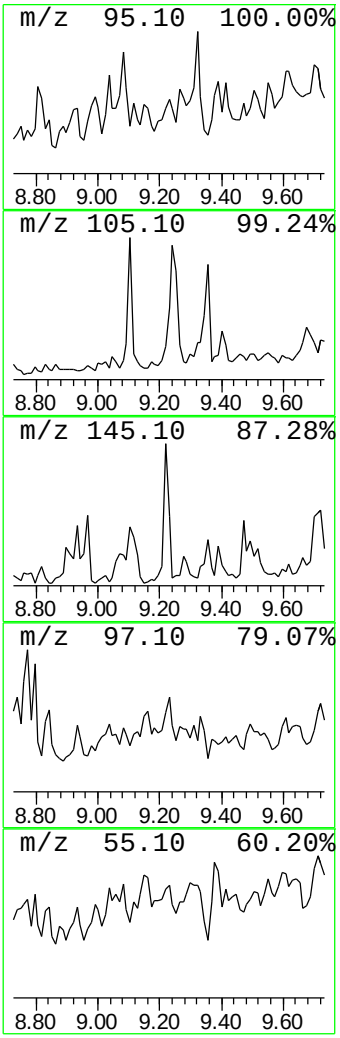
Peak Number 8 unknown9.23 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.23	15.48 ng	880713	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	20
2	Ethanone, 1-[4-(1-methylethenyl)...	160	C11H12O	005359-04-6	20
3	Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	18
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	14
5	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	11





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Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

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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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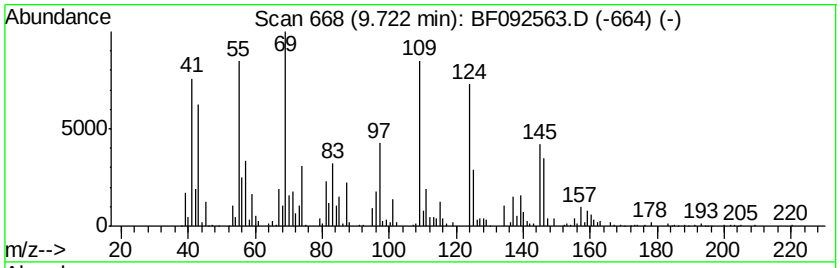
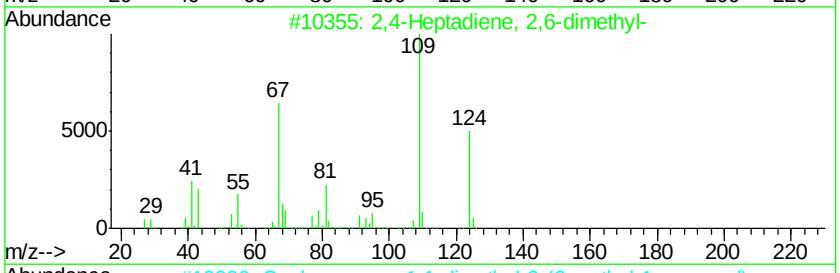
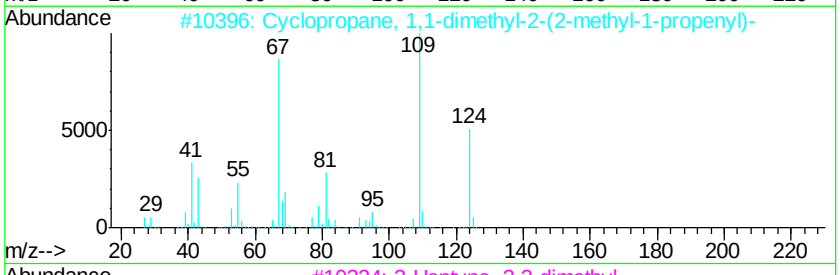
Peak Number 9 unknown9.72 Concentration Rank 4

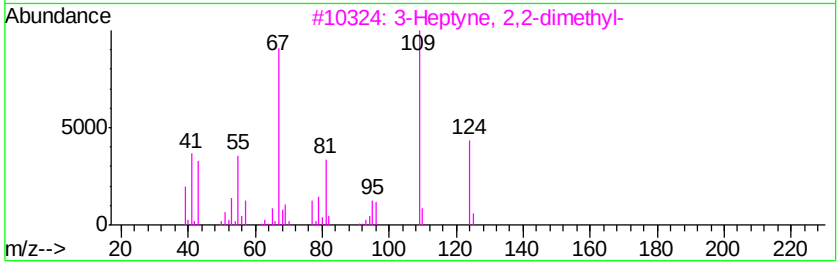
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.72	43.35 ng	2465620	Acenaphthene-d10	10.03

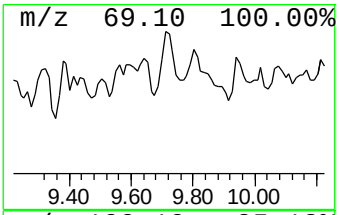
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Heptadiene, 2,6-dimethyl-	124	C9H16	004634-87-1	25
2	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	033422-32-1	22
3	3-Heptyne, 2,2-dimethyl-	124	C9H16	029022-29-5	22
4	Benzenemethanamine, 4-fluoro-	125	C7H8FN	000140-75-0	18
5	Bicyclo[2.2.1]heptan-2-one, 5-hy...	168	C10H16O2	039850-78-7	14

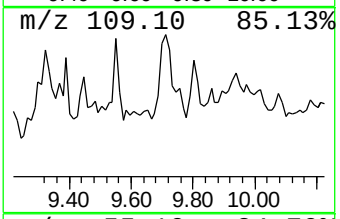


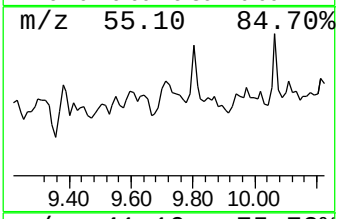


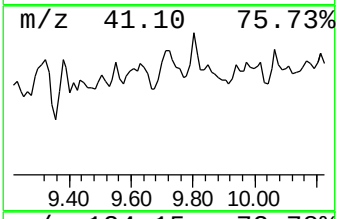


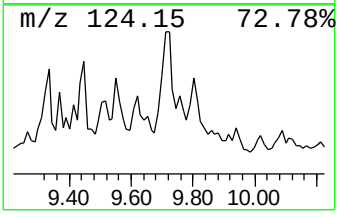












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Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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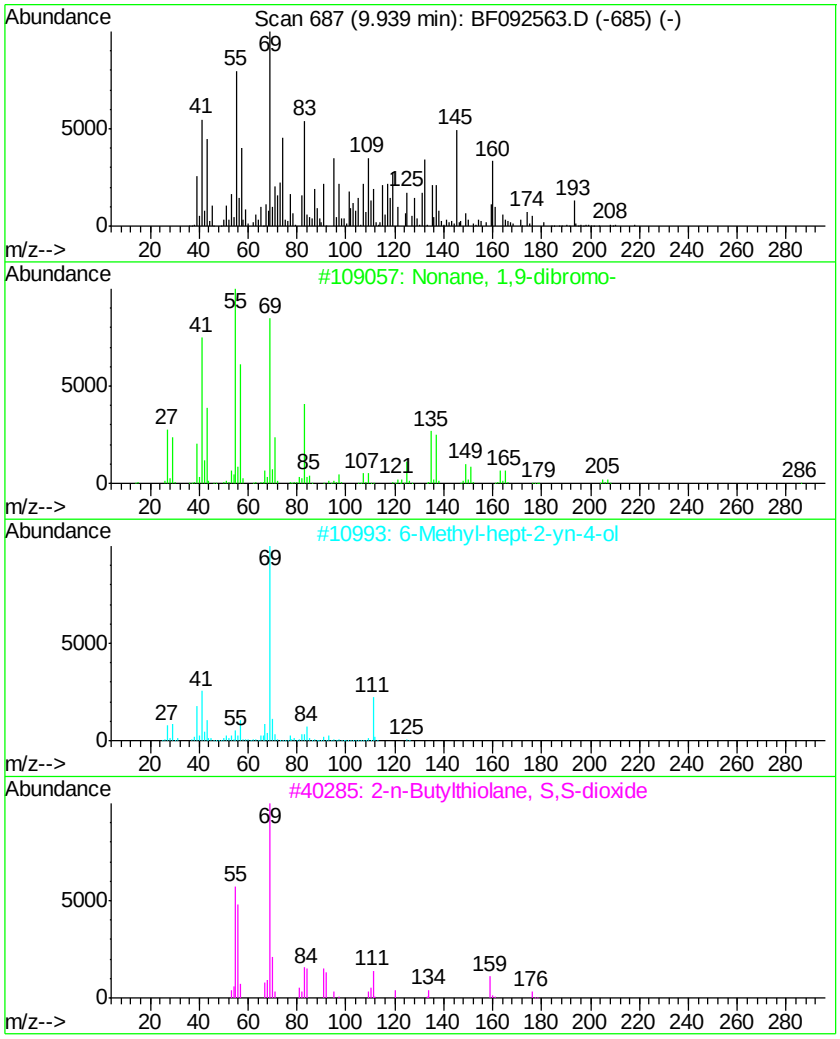
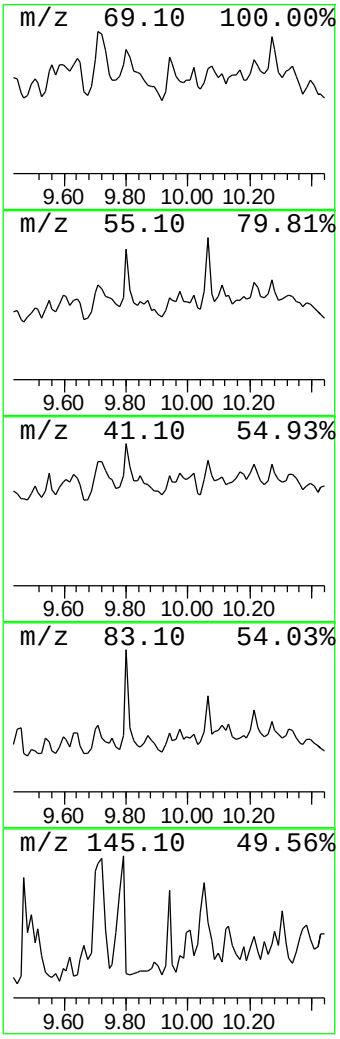
Peak Number 10 unknown9.94 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.94	20.39 ng	1159810	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 1,9-dibromo-	284	C9H18Br2	004549-33-1	35
2	6-Methyl-hept-2-yn-4-ol	126	C8H14O	060018-69-1	22
3	2-n-Butylthiolane, S,S-dioxide	176	C8H16O2S	071053-03-7	22
4	Cyclohexane, 1,1'-(1,2-dimethyl-...	222	C16H30	074663-71-1	22
5	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	22





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Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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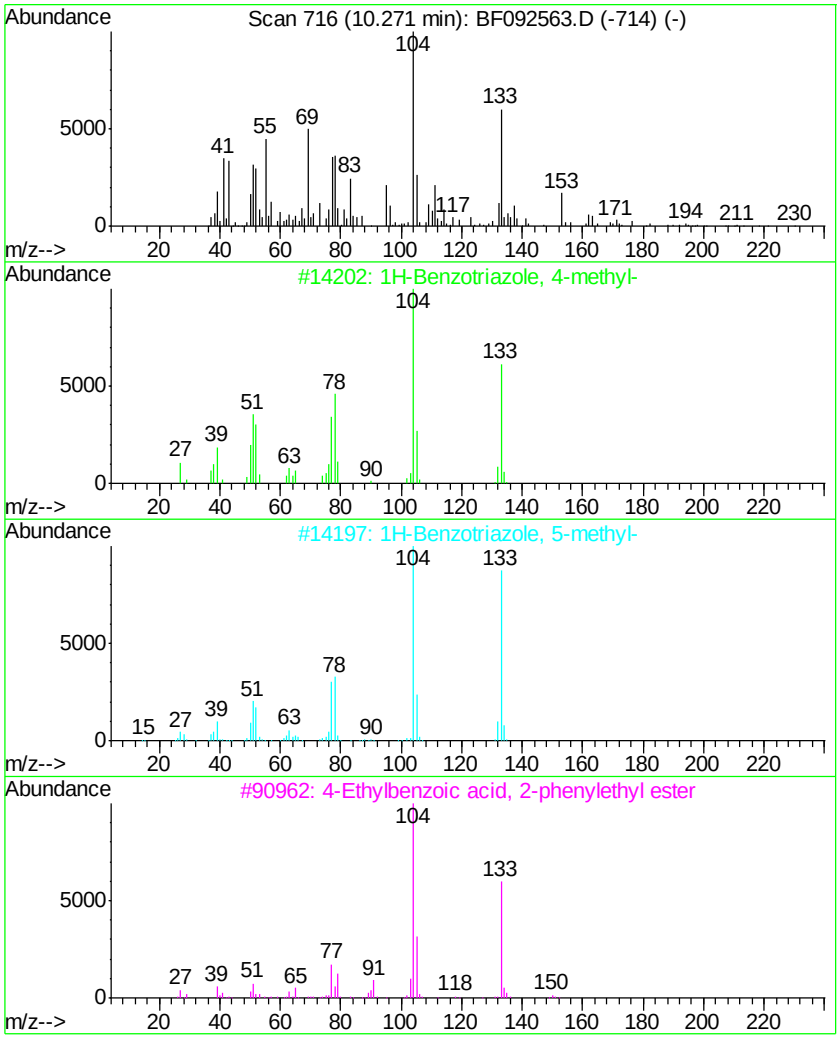
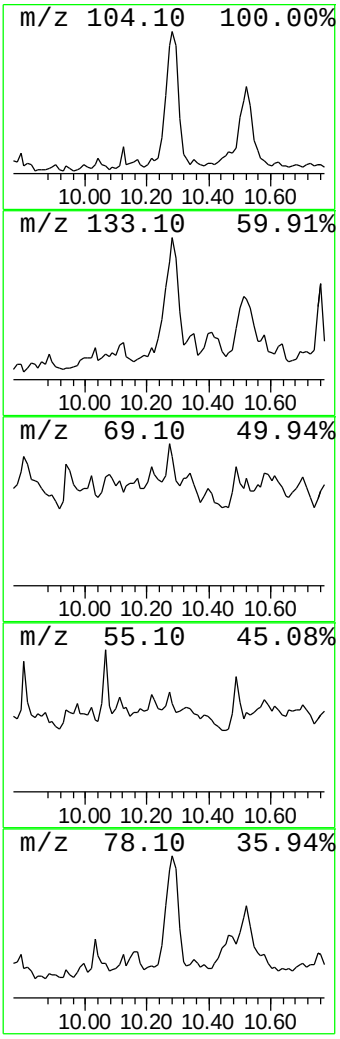
Peak Number 11 1H-Benzotriazole, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	29.15 ng	1658140	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	97
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	93
3	4-Ethylbenzoic acid, 2-phenyleth...	254	C17H18O2	1000293-50-1	27
4	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	20
5	2-Pyridinecarbonitrile	104	C6H4N2	000100-70-9	18





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Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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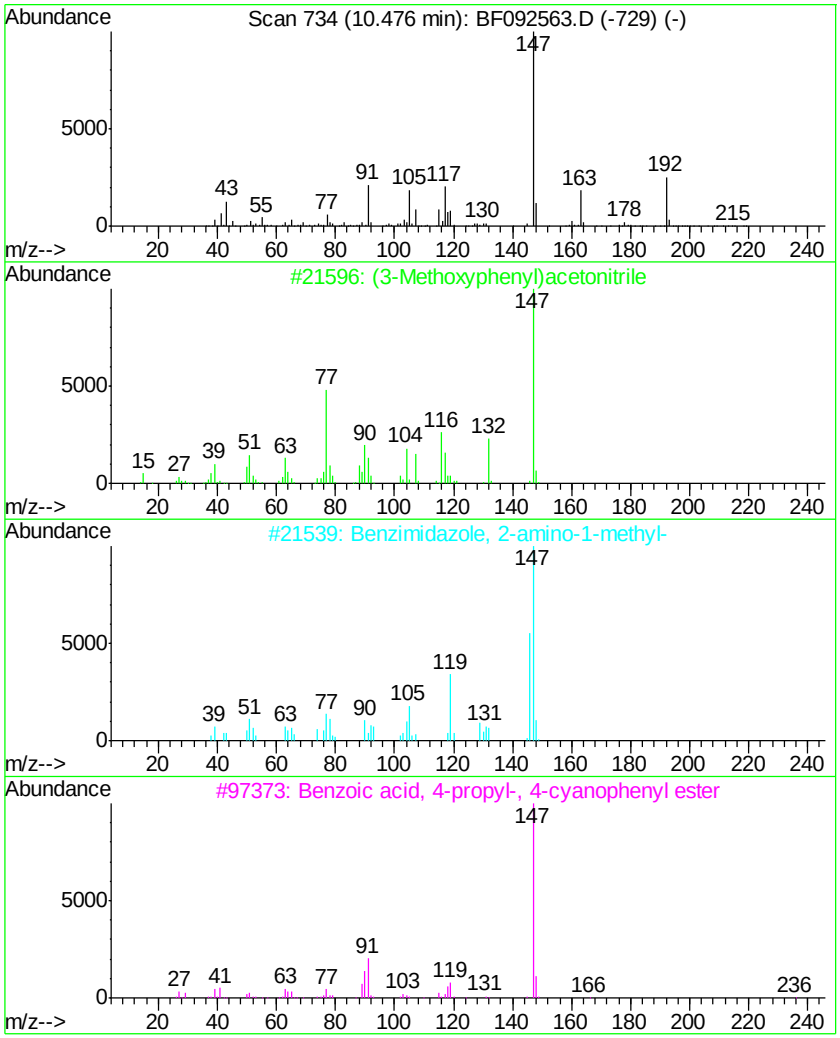
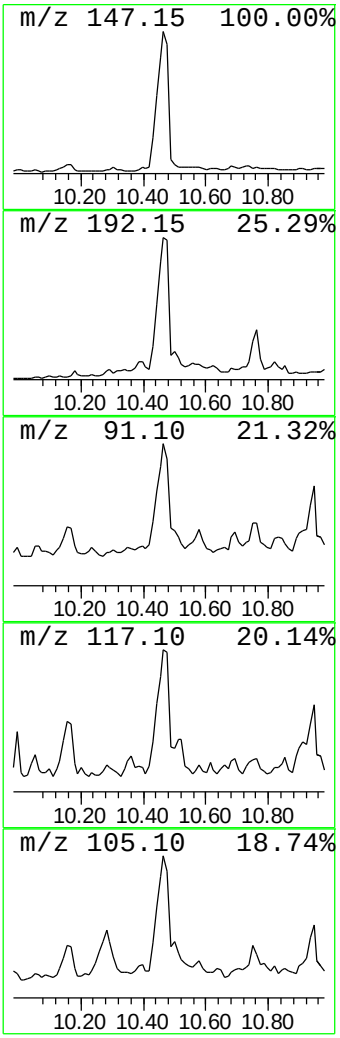
Peak Number 12 (3-Methoxyphenyl)acetonitrile Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.48	120.29 ng	6842560	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3-Methoxyphenyl)acetonitrile	147	C9H9NO	019924-43-7	53
2	Benzimidazole, 2-amino-1-methyl-	147	C8H9N3	001622-57-7	50
3	Benzoic acid, 4-propyl-, 4-cyano...	265	C17H15NO2	056131-49-8	47
4	Benzoic acid, 4-propyl-, 4-cyano...	283	C17H14FNO2	086776-51-4	47
5	o-Diacetylbenzene	162	C10H10O2	000704-00-7	46





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Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

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

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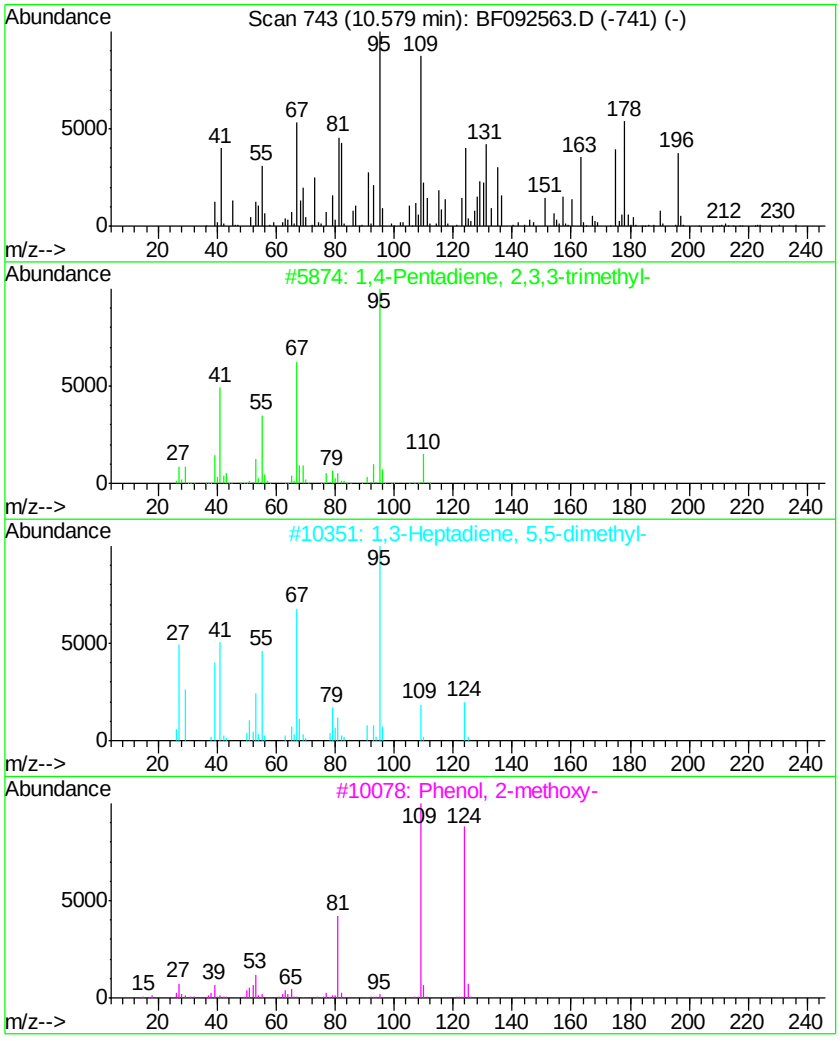
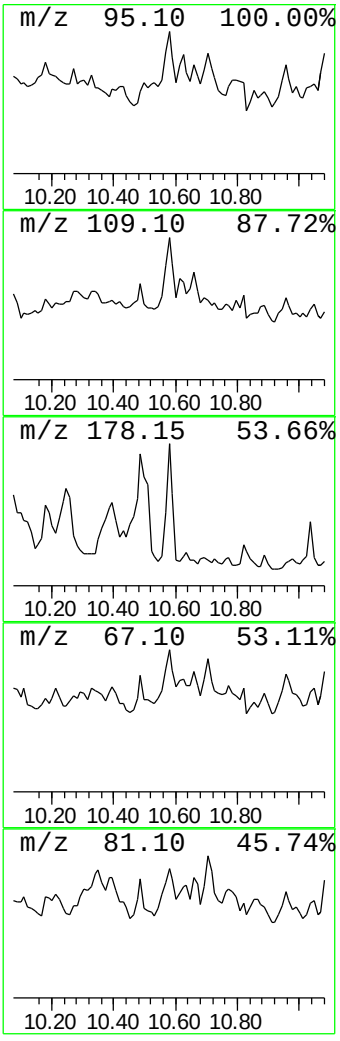
Peak Number 13 unknown10.58 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	21.91 ng	1246140	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	25
2	1,3-Heptadiene, 5,5-dimethyl-	124	C9H16	024618-86-8	25
3	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	20
4	2-Acetyl-5-methylfuran	124	C7H8O2	001193-79-9	18
5	Mequinol	124	C7H8O2	000150-76-5	18





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Instrument : BNA_F
ClientSampleId : MW-03

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

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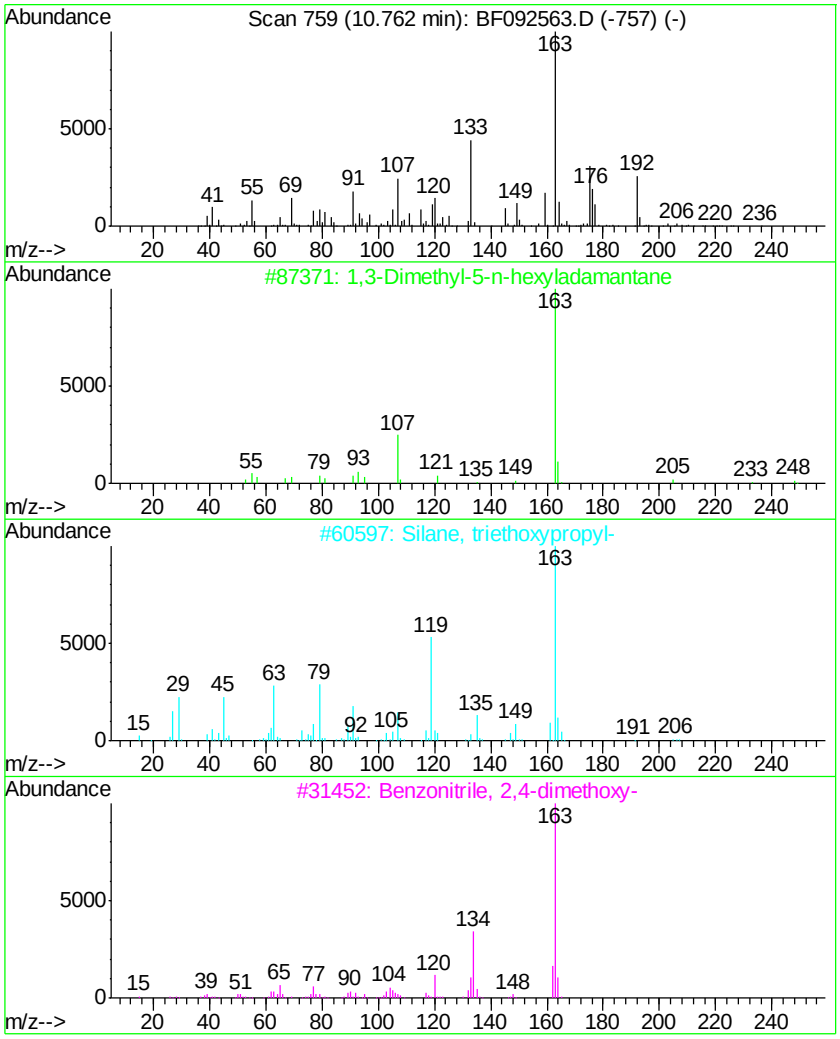
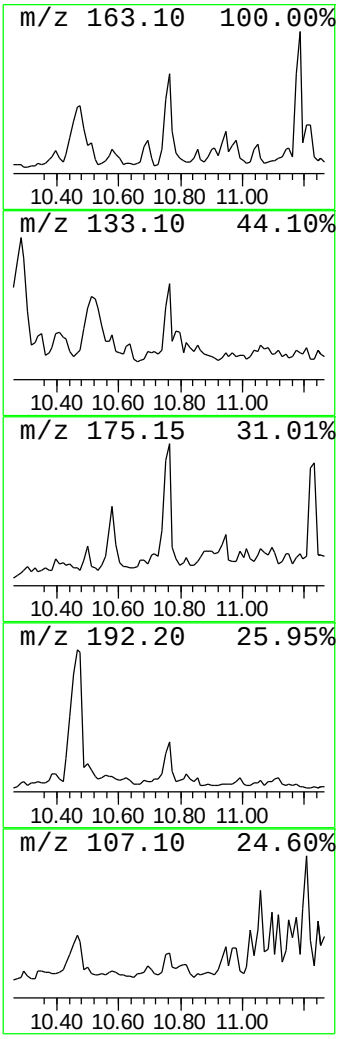
Peak Number 14 unknown10.76 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	23.76 ng	1351730	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethyl-5-n-hexyladamantane	248	C18H32	052873-50-4	35
2	Silane, triethoxypropyl-	206	C9H22O3Si	002550-02-9	35
3	Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	27
4	Benzeneacetic acid, .alpha.,.alp...	209	C10H11NO4	126802-52-6	27
5	1,2-Hexanediol, 1,2-diphenyl-	270	C18H22O2	080475-19-0	27





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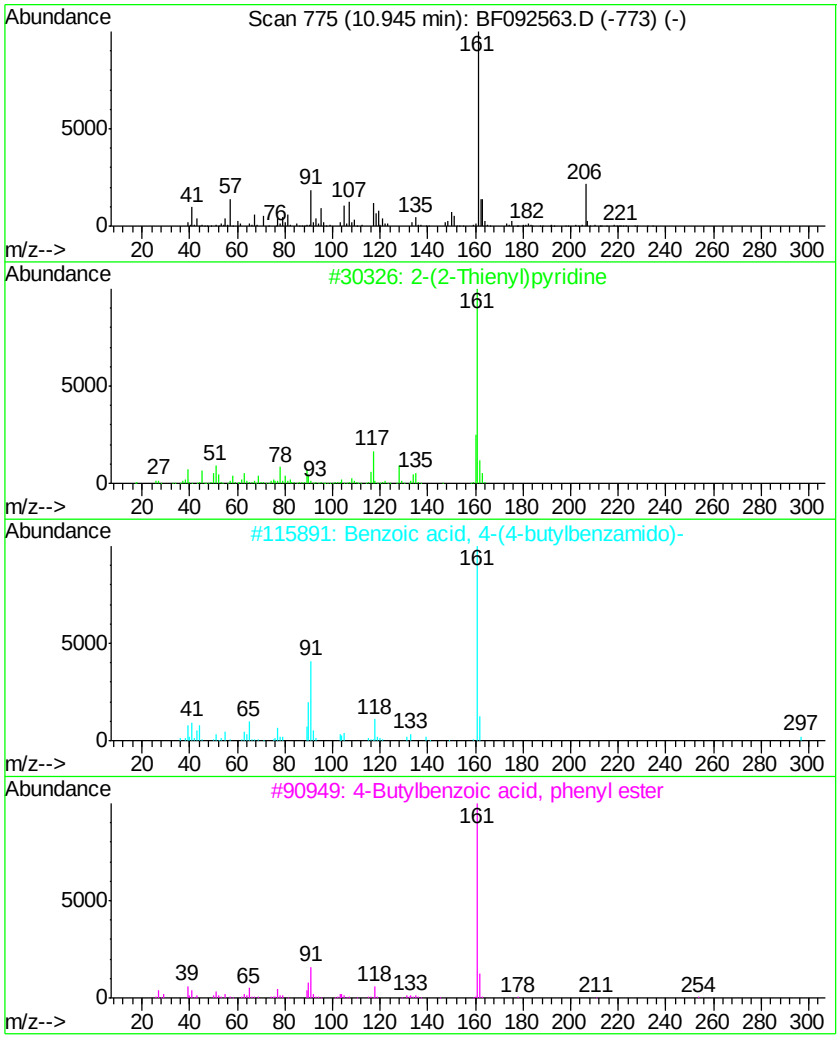
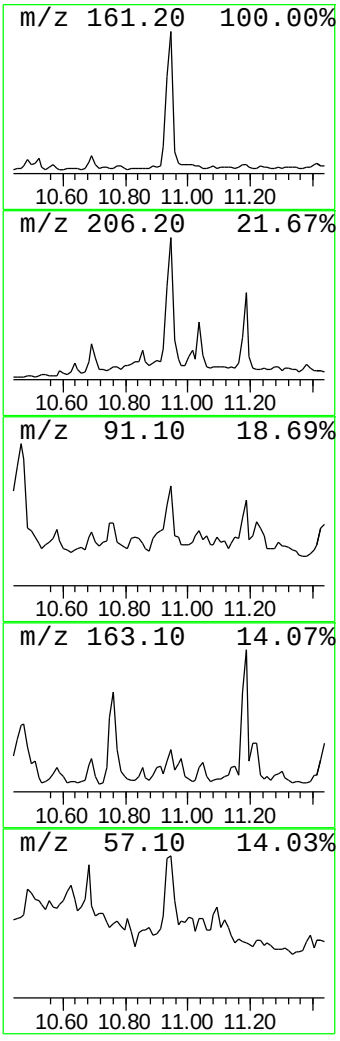
Peak Number 15 2-(2-Thienyl)pyridine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.94	37.63 ng	3069190	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Thienyl)pyridine	161	C9H7NS	003319-99-1	50
2	Benzoic acid, 4-(4-butylbenzamido)-	297	C18H19NO3	313518-53-5	43
3	4-Butylbenzoic acid, phenyl ester	254	C17H18O2	085090-12-6	43
4	4,5,6,7-Tetramethylphthalide	190	C12H14O2	029002-54-8	38
5	4-Phenylpiperidine	161	C11H15N	000771-99-3	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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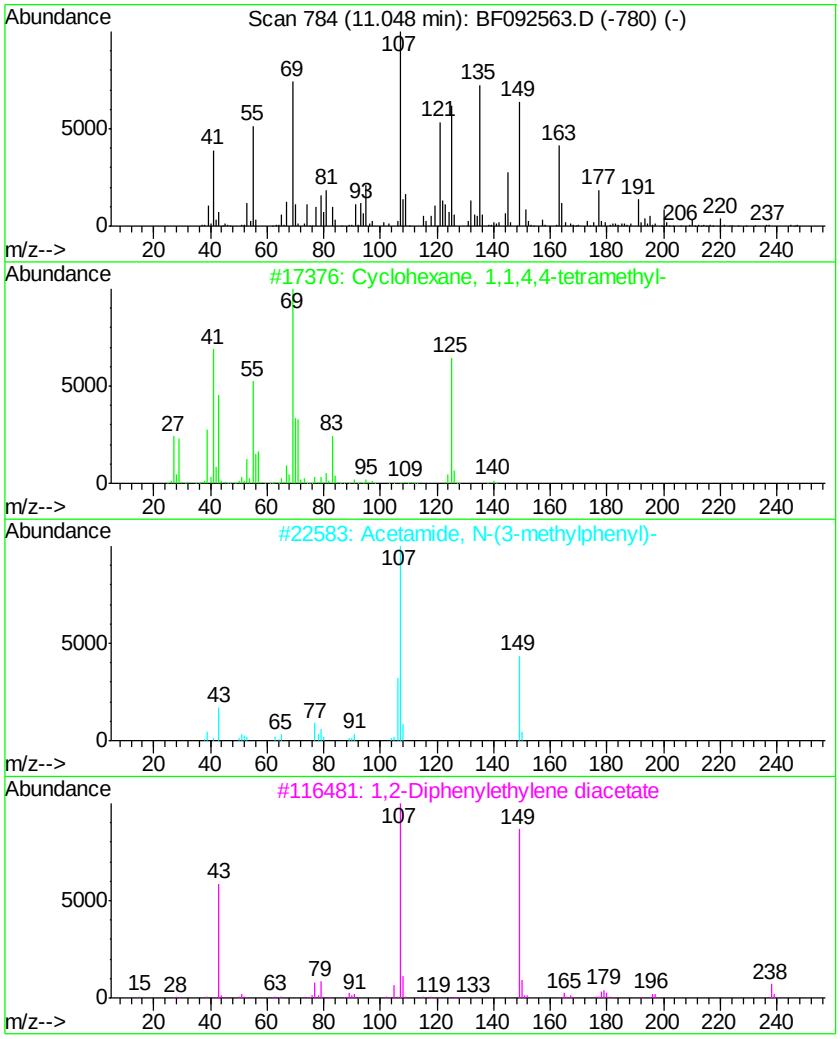
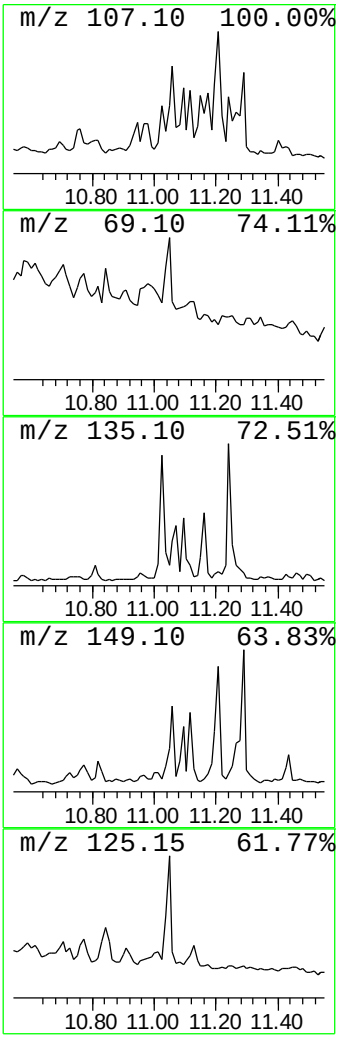
Peak Number 16 unknown11.05 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	29.64 ng	2417560	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,4,4-tetramethyl-	140	C10H20	002223-52-1	18
2	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	14
3	1,2-Diphenylethylene diacetate	298	C18H18O4	003682-07-3	14
4	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	14
5	Cyclooctanecarboxaldehyde	140	C9H16O	006688-11-5	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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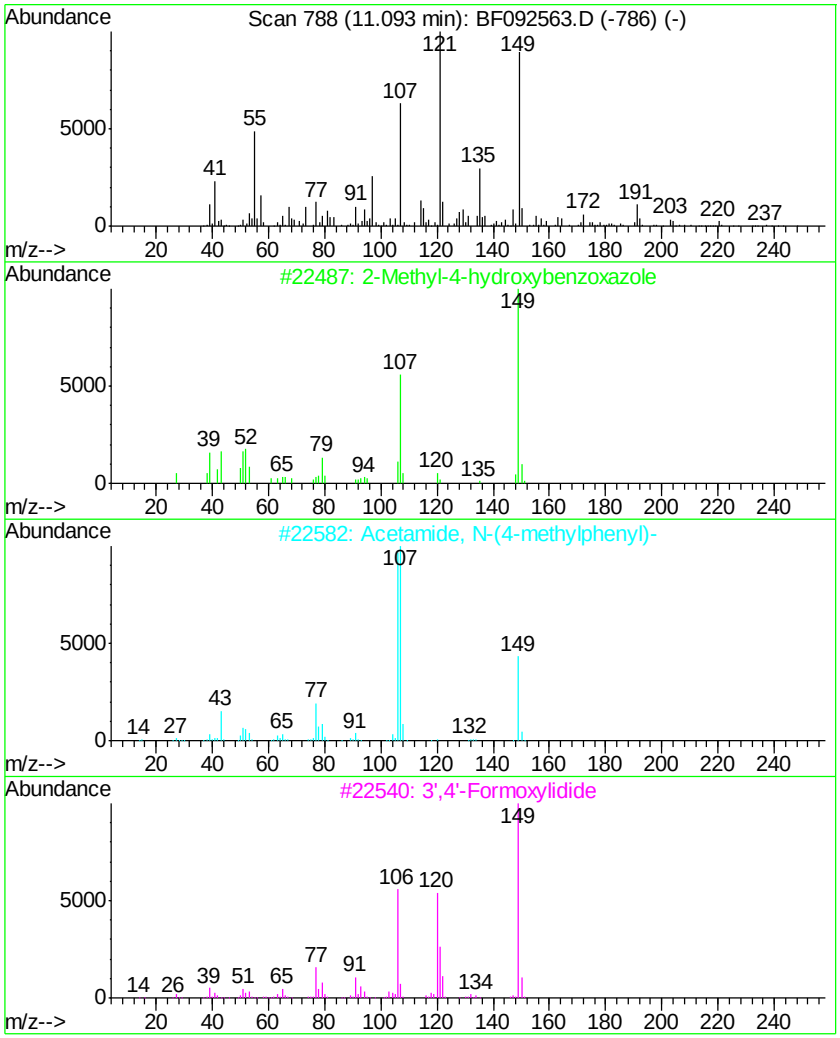
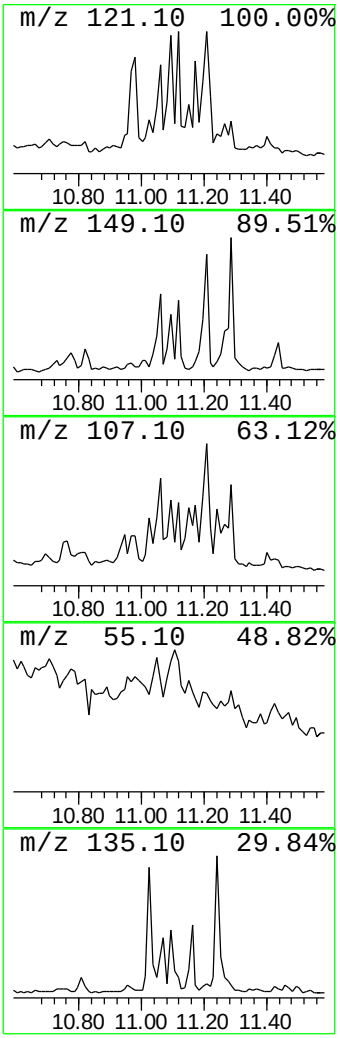
Peak Number 17 unknown11.09 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	26.66 ng	2175050	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	35
2	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	000103-89-9	30
3	3',4'-Formoxylidide	149	C9H11NO	006639-60-7	25
4	Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	25
5	1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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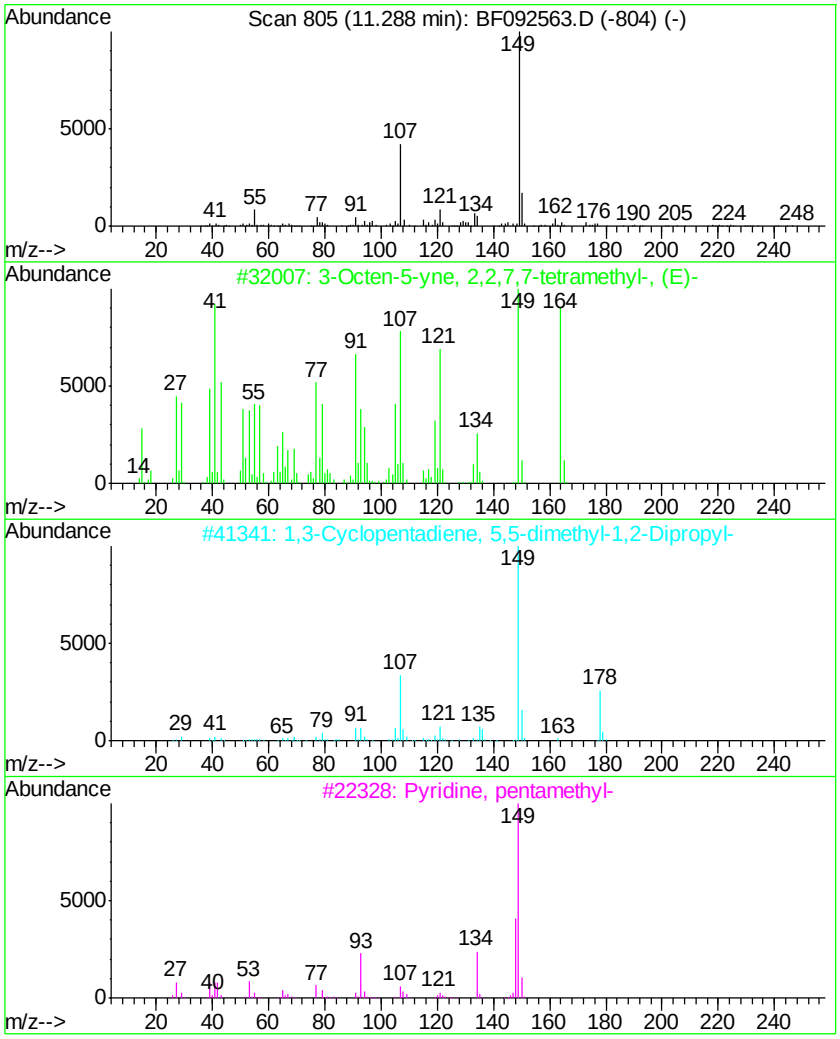
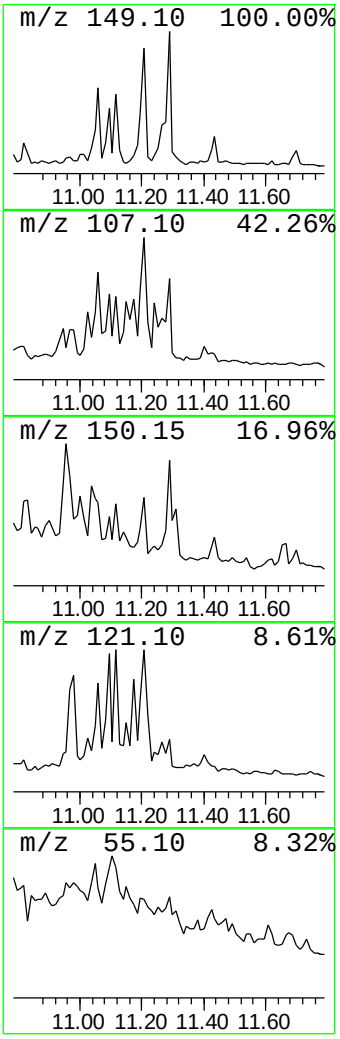
Peak Number 18 3-Octen-5-yne, 2,2,7,7-tetr... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.29	14.11 ng	1150830	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octen-5-yne, 2,2,7,7-tetrameth...	164	C12H20	055976-12-0	72
2	1,3-Cyclopentadiene, 5,5-dimethy...	178	C13H22	1000163-88-0	56
3	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	47
4	7-Methylthieno[3,2-b]pyridine	149	C8H7NS	013362-83-9	47
5	Silane, 1,3-heptadiynyltrimethyl-	164	C10H16Si	019024-47-6	42





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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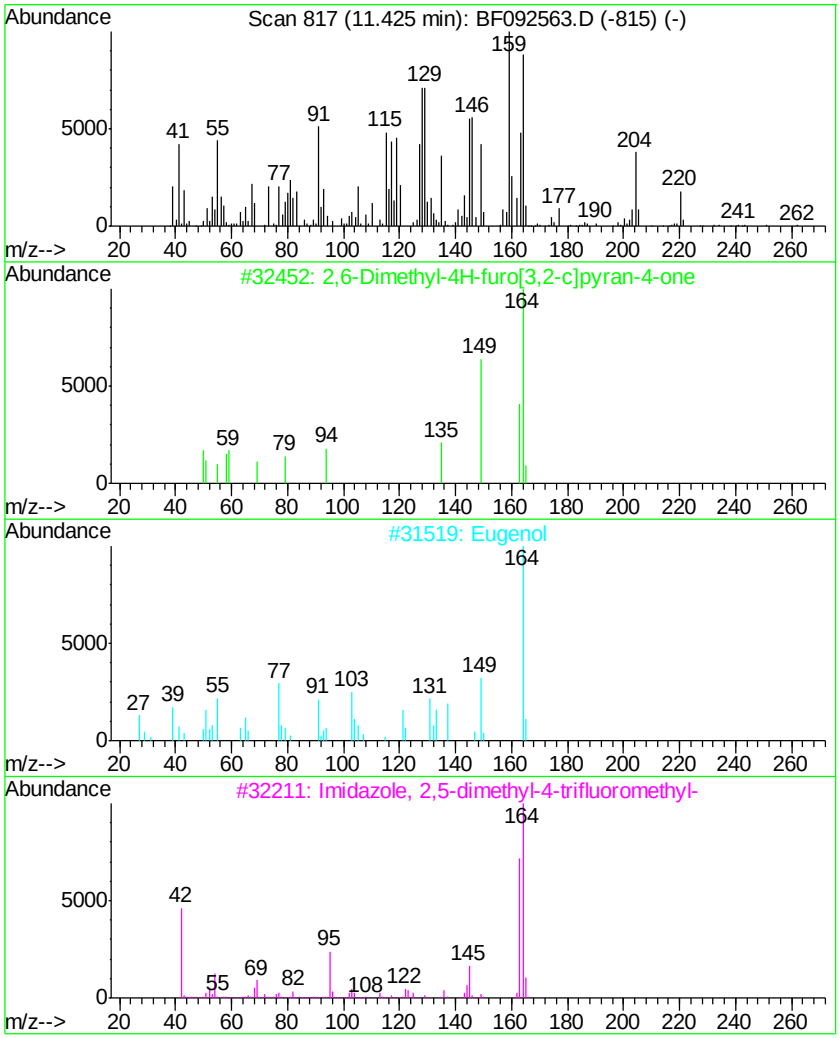
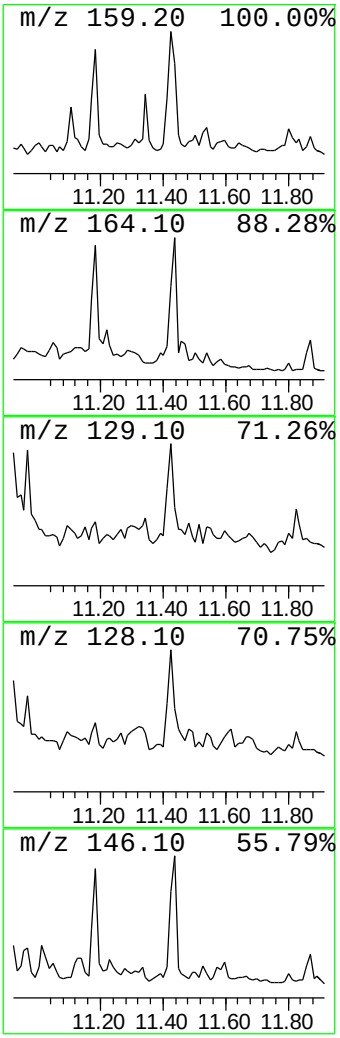
Peak Number 19 unknown11.42 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	18.02 ng	1469860	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-4H-furo[3,2-c]pyran...	164	C9H8O3	087785-58-8	14
2	Eugenol	164	C10H12O2	000097-53-0	11
3	Imidazole, 2,5-dimethyl-4-triflu...	164	C6H7F3N2	081769-62-2	11
4	(.alpha.,.alpha.,.alpha.-Trifluo...	204	C9H7F3O2	032857-62-8	11
5	Methanimidamide, N'-(3-hydroxyph...	164	C9H12N2O	025635-97-6	11





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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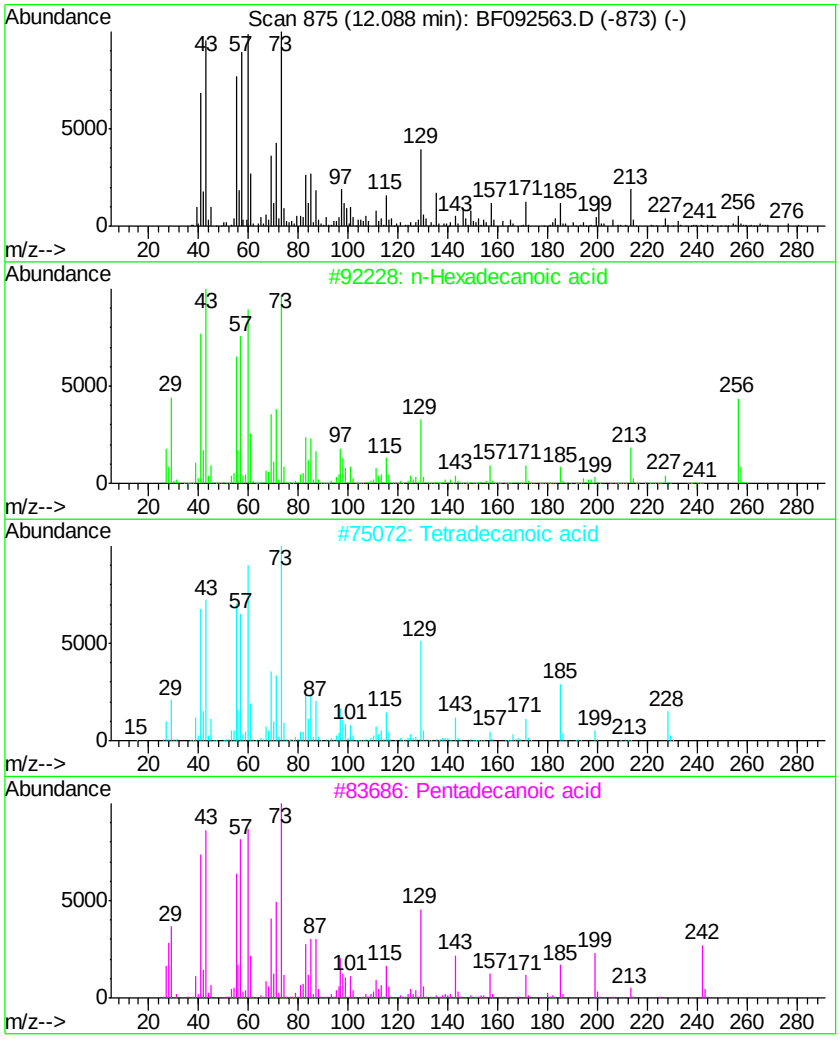
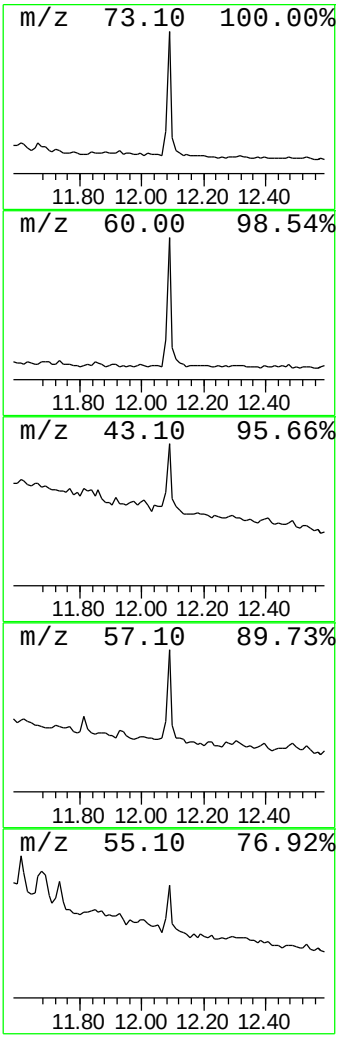
Peak Number 20 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.09	16.44 ng	1341320	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092563.D
Acq On : 27 Jan 2017 8:49
Operator : SJ/MA
Sample : I1353-01
Misc :
ALS Vial : 50 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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
unknown6.74	6.74	56.3	ng	3802240	1	6.97	1350130	20.0
unknown7.41	7.41	11.4	ng	768822	1	6.97	1350130	20.0
Tetrahydrofuran, ...	7.48	13.1	ng	883900	1	6.97	1350130	20.0
unknown8.44	8.44	11.8	ng	1747740	2	8.27	2963170	20.0
2-Propanol, 1-[1-...	8.50	19.0	ng	2815740	2	8.27	2963170	20.0
unknown8.75	8.75	11.5	ng	1705410	2	8.27	2963170	20.0
unknown9.23	9.23	15.5	ng	880713	3	10.03	1137660	20.0
unknown9.72	9.72	43.4	ng	2465620	3	10.03	1137660	20.0
unknown9.94	9.94	20.4	ng	1159810	3	10.03	1137660	20.0
1H-Benzotriazole,...	10.27	29.1	ng	1658140	3	10.03	1137660	20.0
(3-Methoxyphenyl)...	10.48	120.3	ng	6842560	3	10.03	1137660	20.0
unknown10.58	10.58	21.9	ng	1246140	3	10.03	1137660	20.0
unknown10.76	10.76	23.8	ng	1351730	3	10.03	1137660	20.0
2-(2-Thienyl)pyri...	10.94	37.6	ng	3069190	4	11.53	1631410	20.0
unknown11.05	11.05	29.6	ng	2417560	4	11.53	1631410	20.0
unknown11.09	11.09	26.7	ng	2175050	4	11.53	1631410	20.0
3-Octen-5-yne, 2,...	11.29	14.1	ng	1150830	4	11.53	1631410	20.0
unknown11.42	11.42	18.0	ng	1469860	4	11.53	1631410	20.0
n-Hexadecanoic acid	12.09	16.4	ng	1341320	4	11.53	1631410	20.0