LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092511.D
Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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	2.510	35	37	49	rVB2	21966	63168	1.57%	0.132%
2	3.184	93	96	103	rVB	114102	218413	5.44%	0.457%
3	3.744	140	145	151	rBV2	38533	86304	2.15%	0.180%
4	3.847	151	154	157	rBV	32834	52003	1.30%	0.109%
5	4.236	184	188	191	rBV2	21632	47816	1.19%	0.100%
6	4.407	198	203	204	rBV3	38659	114738	2.86%	0.240%
7	4.533	210	214	216	rBV2	30643	67027	1.67%	0.140%
8	4.590	216	219	224	rVB2	74255	116018	2.89%	0.243%
9	5.047	253	259	261	rBV4	28997	96914	2.41%	0.203%
10	5.150	265	268	271	rVV	407975	630080	15.69%	1.318%
11	5.207	271	273	277	rVV2	97388	177073	4.41%	0.370%
12	5.276	277	279	282	rVB	160362	158801	3.95%	0.332%
13	5.561	301	304	306	rBV	1965472	2148803	53.51%	4.494%
14	5.619	307	309	310	rBV	77118	62652	1.56%	0.131%
15	5.744	317	320	322	rBV	92334	136552	3.40%	0.286%
16	5.813	324	326	327	rBV2	56846	102780	2.56%	0.215%
17	5.870	329	331	333	rVV2	71358	115001	2.86%	0.241%
18	5.904	333	334	338	rVB3	54845	81069	2.02%	0.170%
19	6.007	338	343	344	rBV3	59039	160649	4.00%	0.336%
20	6.202	358	360	364	rVB	64511	104607	2.61%	0.219%
21	6.293	364	368	369	rBV2	96549	125566	3.13%	0.263%
22	6.327	369	371	372	rVB2	51620	58254	1.45%	0.122%
23	6.396	375	377	379	rVB	117187	160652	4.00%	0.336%
24	6.476	379	384	385	rBV3	50206	117682	2.93%	0.246%
25	6.579	391	393	397	rVB	1157006	1603988	39.95%	3.355%
26	6.727	404	406	409	rBV	2564507	3468837	86.39%	7.255%
27	6.773	409	410	412	rVB2	81350	91314	2.27%	0.191%
28	6.922	420	423	425	rBV2	47473	73552	1.83%	0.154%
29	6.967	425	427	428	rVV	1108834	943985	23.51%	1.974%
30	7.002	428	430	431	rVV	405787	430270	10.72%	0.900%
31	7.047	431	434	436	rVB4	26308	60156	1.50%	0.126%
32	7.127	438	441	443	rVV	3307033	3214133	80.05%	6.722%
33	7.162	443	444	446	rVV2	192078	348181	8.67%	0.728%
34	7.242	446	451	453	rVB2	350487	994225	24.76%	2.079%

LSC Area Percent Report

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Acq On : 26 Jan 2017 8:35
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Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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

35	7.299	453	456	460	rBV4	40390	123052	3.06%	0.257%
36	7.367	460	462	464	rVB2	64710	61038	1.52%	0.128%
37	7.402	464	465	469	rVB3	47390	97398	2.43%	0.204%
38	7.482	469	472	473	rBV	174343	253946	6.32%	0.531%
39	7.539	473	477	478	rVV	2494988	3765516	93.78%	7.875%
40	7.562	478	479	481	rVV	699269	1284607	31.99%	2.687%
41	7.596	481	482	486	rVB	711549	700807	17.45%	1.466%
42	7.665	486	488	489	rBV2	71707	117147	2.92%	0.245%
43	7.790	497	499	500	rBV	131308	151213	3.77%	0.316%
44	7.836	500	503	506	rVV3	289790	610428	15.20%	1.277%
45	7.893	506	508	509	rVV2	48272	70780	1.76%	0.148%
46	7.916	509	510	514	rVB3	154407	196877	4.90%	0.412%
47	7.973	514	515	516	rBV	44686	49615	1.24%	0.104%
48	8.019	516	519	521	rVV2	79158	127230	3.17%	0.266%
49	8.065	521	523	528	rVB4	53582	95859	2.39%	0.200%
50	8.179	528	533	534	rBV2	177528	288543	7.19%	0.603%
51	8.259	537	540	542	rBV	1364427	1281710	31.92%	2.681%
52	8.327	544	546	551	rVB4	76164	134892	3.36%	0.282%
53	8.419	551	554	555	rBV3	65954	127997	3.19%	0.268%
54	8.453	555	557	561	rVV2	273244	486972	12.13%	1.018%
55	8.522	561	563	565	rVV	784414	745781	18.57%	1.560%
56	8.567	565	567	568	rVV2	35486	65056	1.62%	0.136%
57	8.602	568	570	575	rVB3	103300	157792	3.93%	0.330%
58	8.682	575	577	578	rBV2	50421	79956	1.99%	0.167%
59	8.739	579	582	584	rVB3	174839	238192	5.93%	0.498%
60	8.785	584	586	587	rBV	220844	244441	6.09%	0.511%
61	8.853	590	592	594	rBV	155350	172810	4.30%	0.361%
62	8.910	596	597	598	rVV	85557	62756	1.56%	0.131%
63	8.968	600	602	604	rVV2	132653	230792	5.75%	0.483%
64	9.036	606	608	609	rBV	73914	108858	2.71%	0.228%
65	9.070	609	611	612	rVV	302171	307675	7.66%	0.643%
66	9.116	614	615	617	rVV2	321266	312951	7.79%	0.655%
67	9.150	617	618	620	rVB	141341	122580	3.05%	0.256%
68	9.208	620	623	625	rBV2	227618	375741	9.36%	0.786%
69	9.242	625	626	627	rVV	139017	102881	2.56%	0.215%
70	9.276	627	629	630	rVV2	47608	81945	2.04%	0.171%
71	9.345	632	635	637	rVV	4033126	3988289	99.33%	8.341%

LSC Area Percent Report

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Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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	9.390	637	639	641	rVV3	74203	122679	3.06%	0.257%
73	9.436	641	643	646	rVB2	123793	172152	4.29%	0.360%
74	9.505	646	649	650	rBV3	102595	160923	4.01%	0.337%
75	9.528	650	651	653	rVB	195458	159034	3.96%	0.333%
76	9.585	653	656	661	rBV5	163681	277841	6.92%	0.581%
77	9.653	661	662	668	rVB3	128879	271616	6.76%	0.568%
78	9.870	676	681	683	rBV	267992	312739	7.79%	0.654%
79	9.905	683	684	686	rBV2	115218	173004	4.31%	0.362%
80	10.030	692	695	696	rVB	1016759	1318191	32.83%	2.757%
81	10.065	696	698	701	rVB3	106133	229998	5.73%	0.481%
82	10.133	701	704	707	rVB3	53579	135904	3.38%	0.284%
83	10.191	707	709	711	rBV2	101886	139553	3.48%	0.292%
84	10.236	711	713	715	rVB3	44999	56557	1.41%	0.118%
85	10.385	724	726	729	rVB2	36055	65713	1.64%	0.137%
86	10.442	729	731	734	rBV3	38370	78445	1.95%	0.164%
87	10.762	755	759	761	rVB4	21334	61605	1.53%	0.129%
88	10.819	761	764	766	rBV	2233213	2558104	63.71%	5.350%
89	10.933	772	774	777	rVB2	59521	77184	1.92%	0.161%
90	11.173	793	795	798	rVB3	26059	51625	1.29%	0.108%
91	11.379	811	813	818	rVB2	55428	91566	2.28%	0.192%
92	11.516	822	825	827	rBV	1199600	1317415	32.81%	2.755%
93	12.042	868	871	873	rBV	74473	88943	2.22%	0.186%
94	13.105	961	964	966	rBV	3833511	4015387	100.00%	8.398%
95	13.939	1034	1037	1038	rBV	31588	48843	1.22%	0.102%
96	13.962	1038	1039	1041	rVV	113452	90691	2.26%	0.190%
97	14.145	1053	1055	1058	rBV	981580	934405	23.27%	1.954%
98	15.014	1129	1131	1137	rVB3	24553	46346	1.15%	0.097%
99	15.620	1181	1184	1187	rBV	570821	829210	20.65%	1.734%
100	17.300	1328	1331	1339	rVB5	32133	73018	1.82%	0.153%

Sum of corrected areas: 47814077

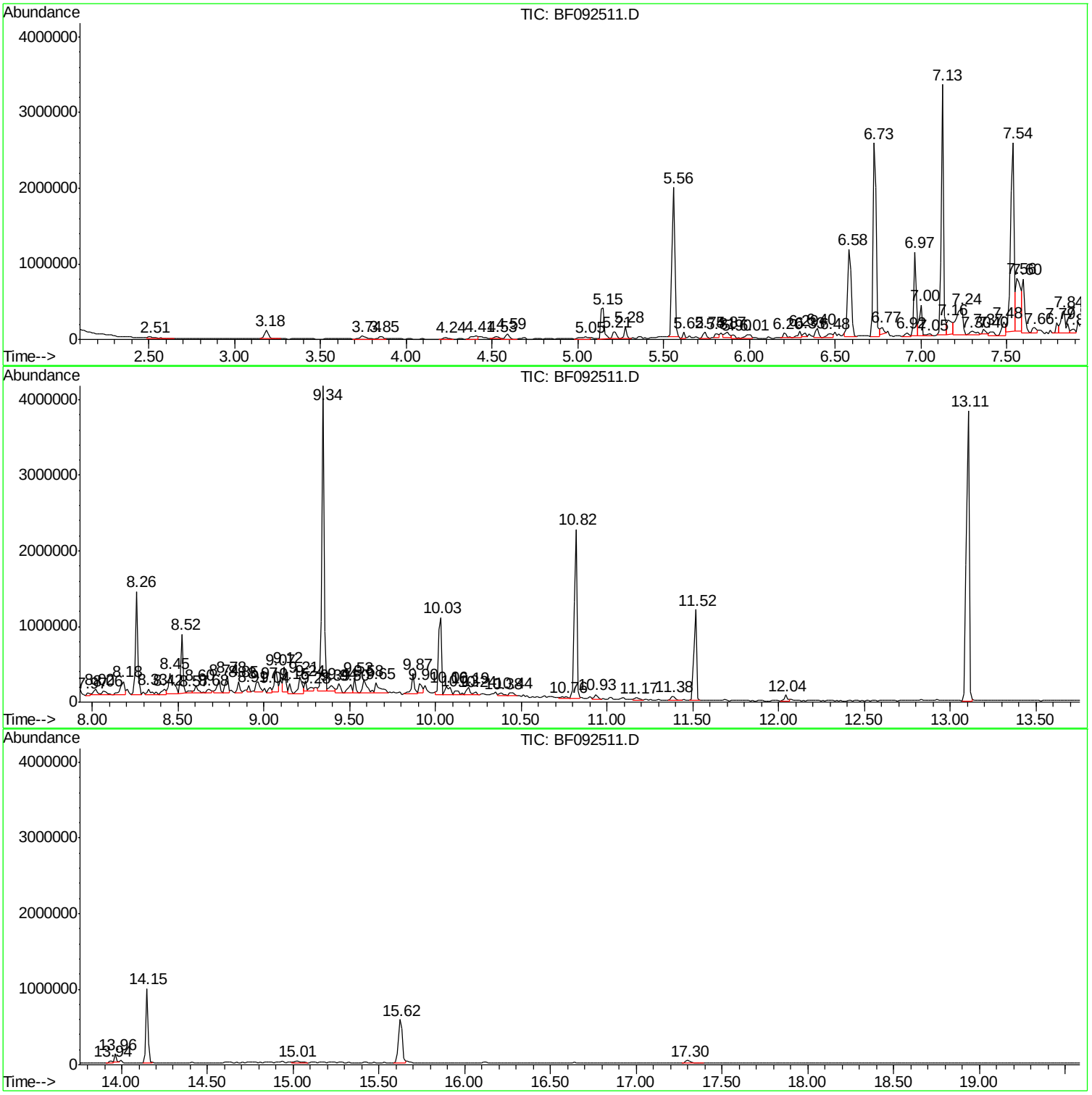
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092511.D
Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5A-012017

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 : BF092511.D
Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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

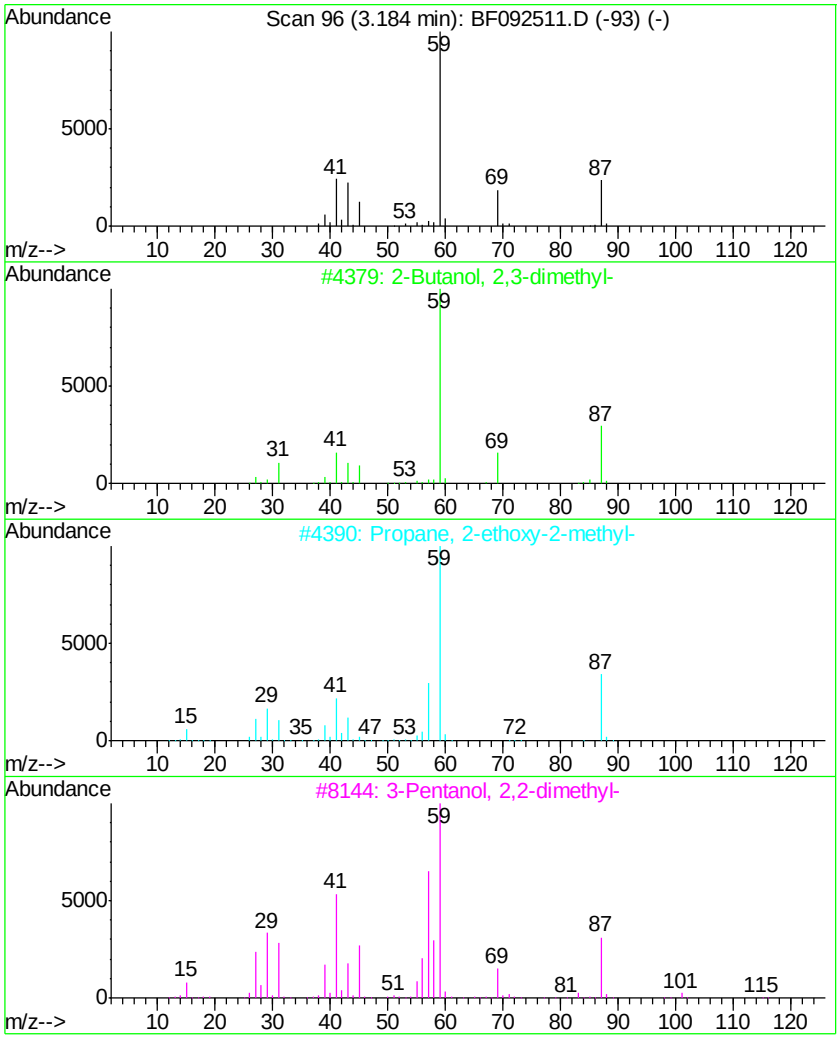
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

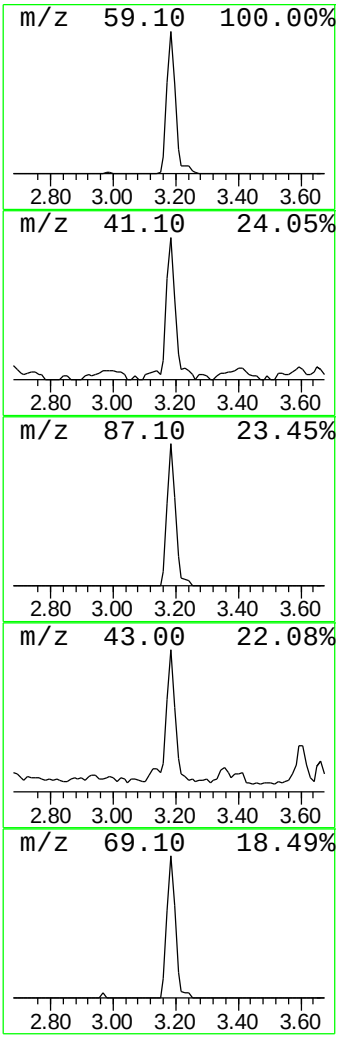
****

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	4.63 ng	218413	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	78
2	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40
4	3-Heptanol	116	C7H16O	000589-82-2	39
5	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	39





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092511.D
Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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

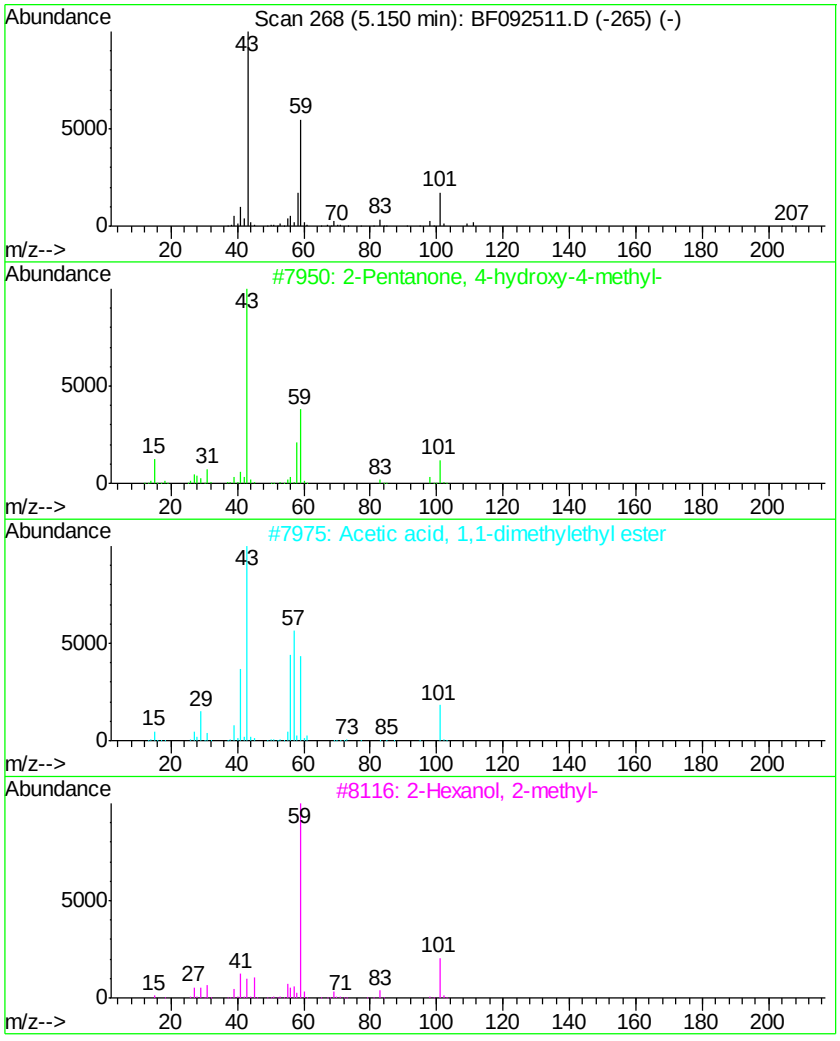
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

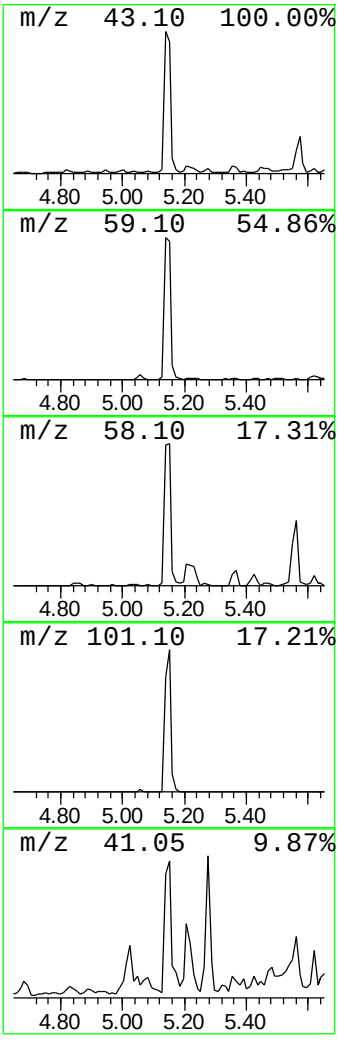
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	13.35 ng	630080	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	37
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument : BNA_F
ClientSampleId : MW-5A-012017

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

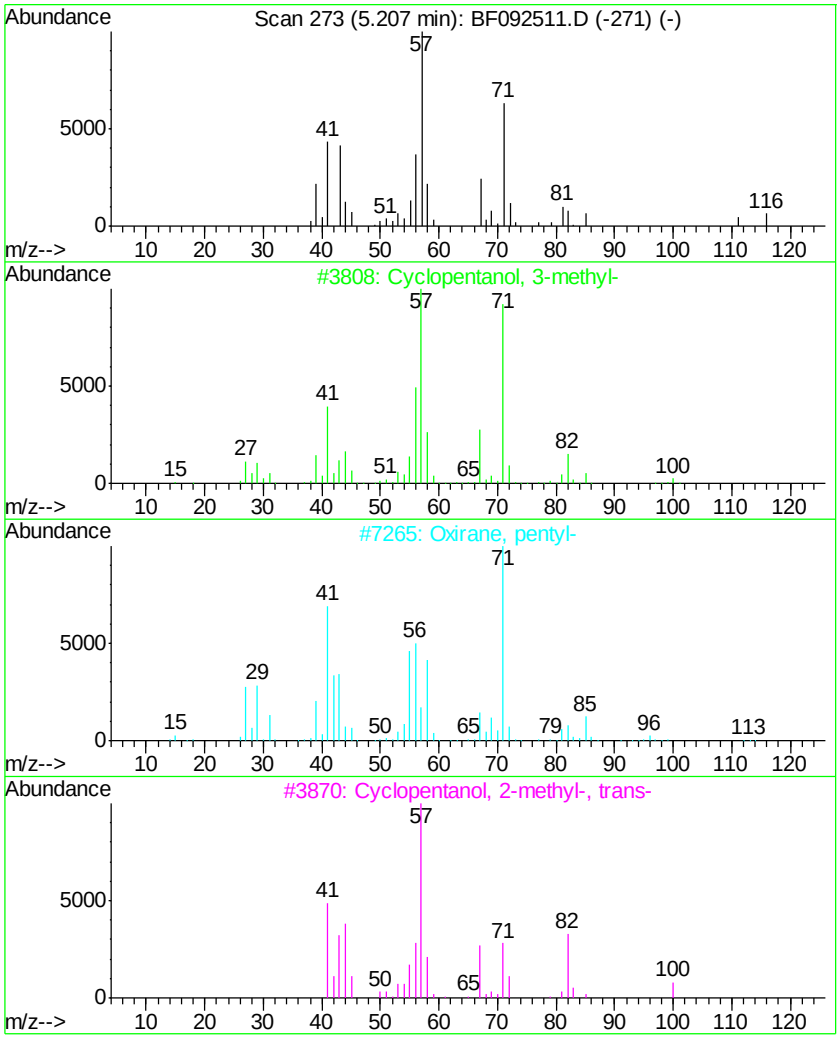
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

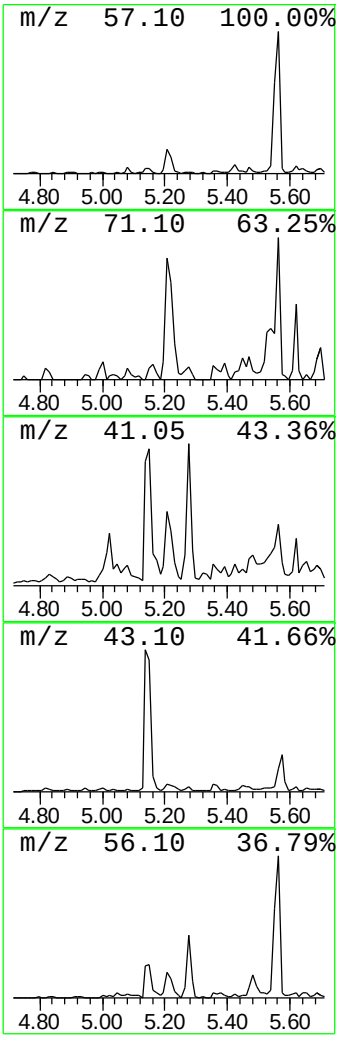
****

Peak Number 3 Cyclopentanol, 3-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	3.75 ng	177073	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanol, 3-methyl-	100	C6H12O	018729-48-1	64
2	Oxirane, pentyl-	114	C7H14O	005063-65-0	40
3	Cyclopentanol, 2-methyl-, trans-	100	C6H12O	025144-04-1	37
4	Cyclopentanol, 2-methyl-	100	C6H12O	024070-77-7	33
5	3-Bromooctane	192	C8H17Br	000999-64-4	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
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Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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

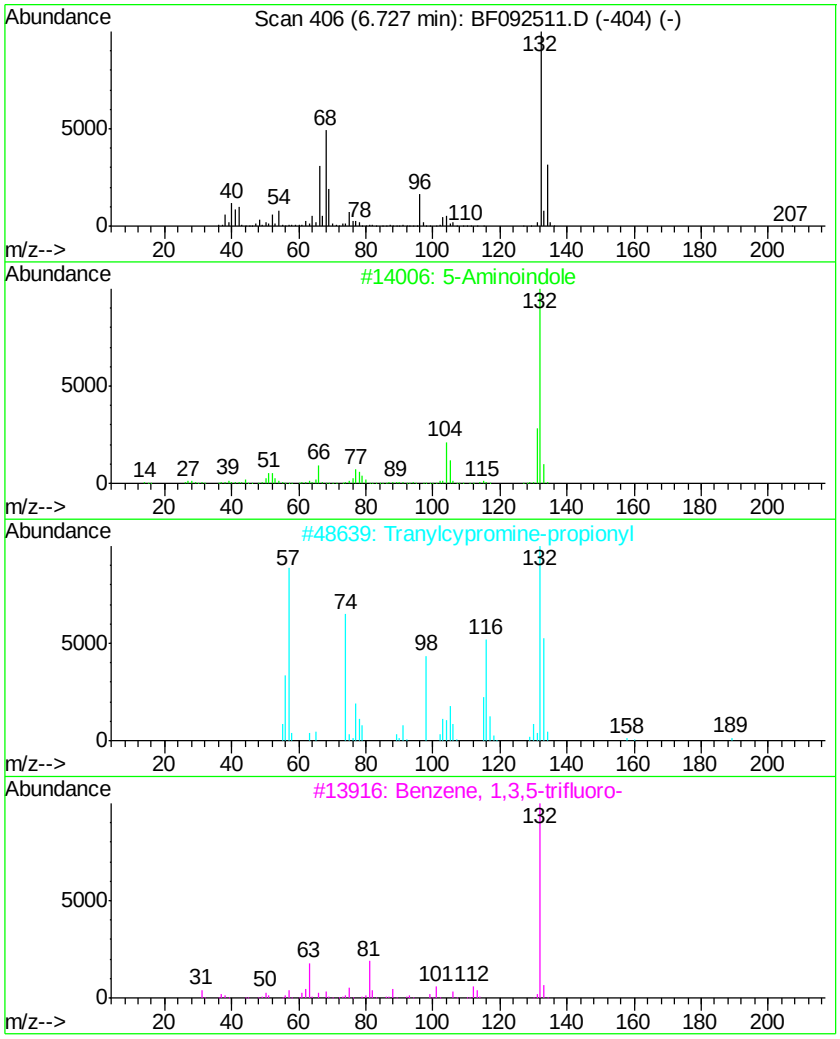
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

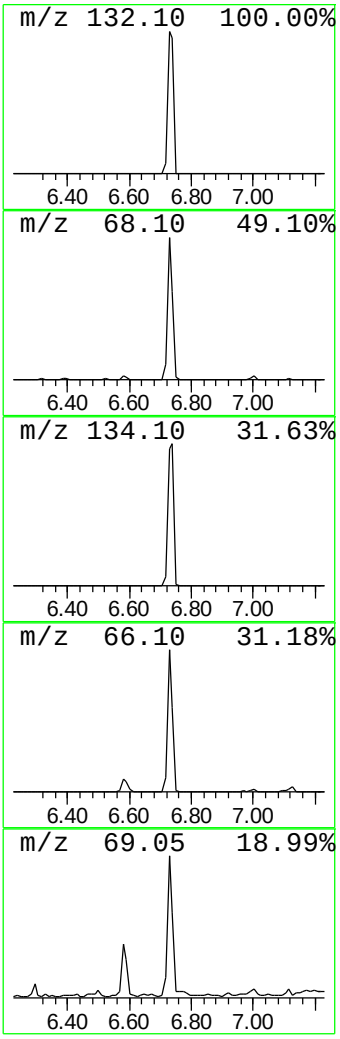
****

Peak Number 4 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	73.49 ng	3468840	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Data File : BF092511.D
Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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

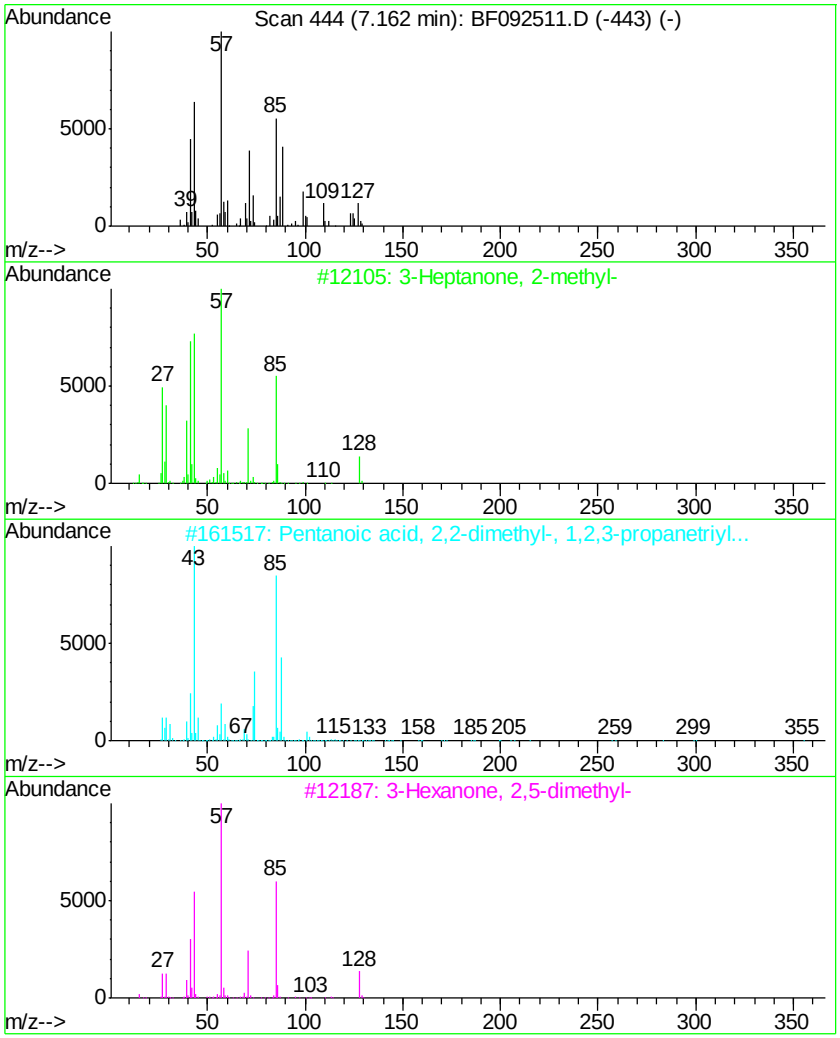
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

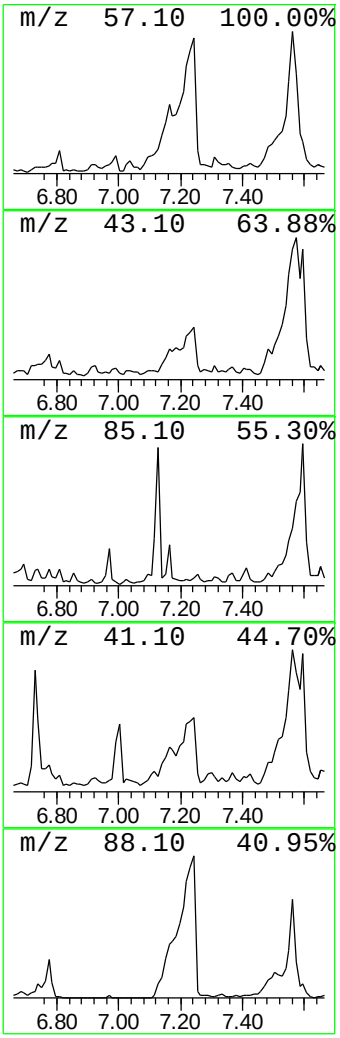
****

Peak Number 6 unknown7.16 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	7.38 ng	348181	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptanone, 2-methyl-	128	C8H16O	013019-20-0	43
2	Pentanoic acid, 2,2-dimethyl-, 1...	428	C24H44O6	057346-62-0	38
3	3-Hexanone, 2,5-dimethyl-	128	C8H16O	001888-57-9	27
4	Heptane, 4-ethyl-	128	C9H20	002216-32-2	22
5	Pentanoic acid, butyl ester	158	C9H18O2	000591-68-4	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092511.D
Acq On : 26 Jan 2017 8:35
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Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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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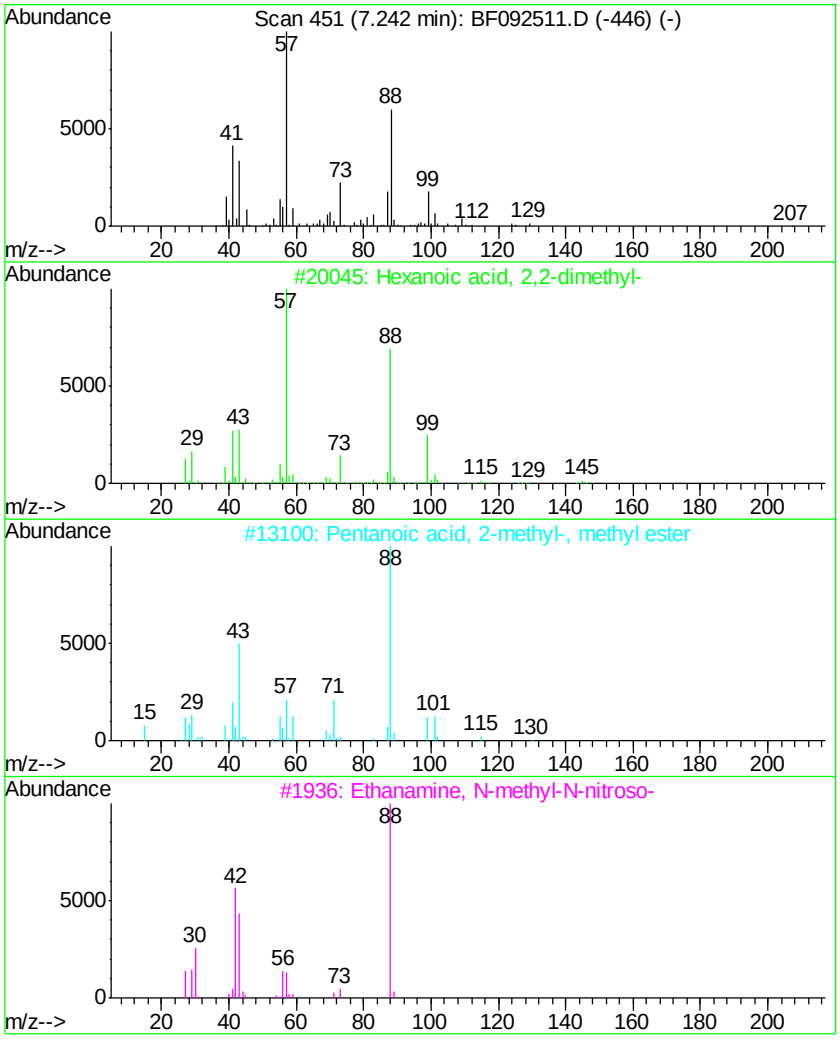
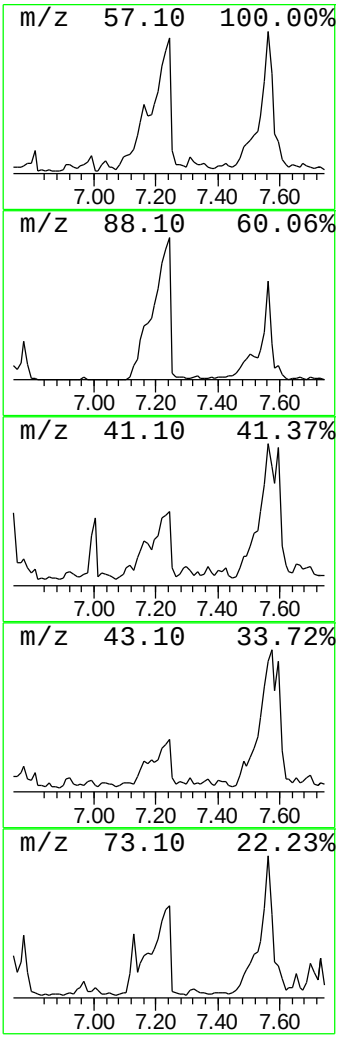
Peak Number 7 Hexanoic acid, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.24	21.06 ng	994225	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	53
2	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	37
3	Ethanamine, N-methyl-N-nitroso-	88	C3H8N2O	010595-95-6	35
4	Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	35
5	Butanoic acid, 2,2-diethyl-	144	C8H16O2	000813-58-1	25





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092511.D
Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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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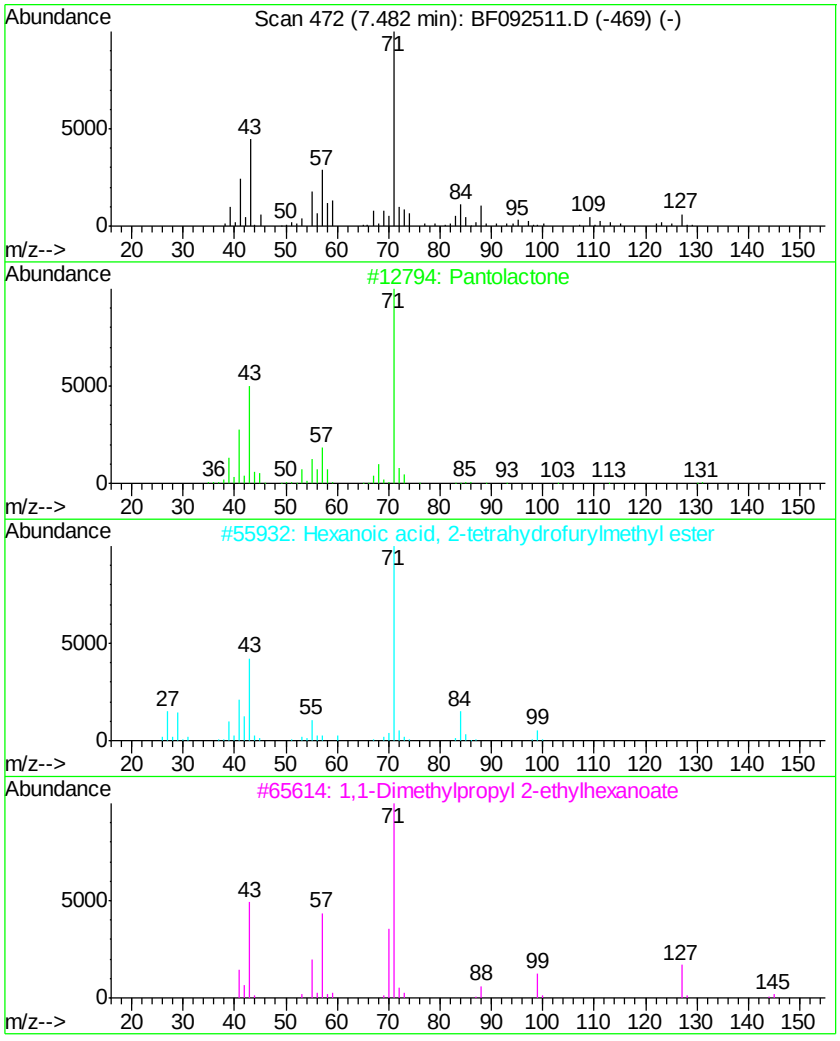
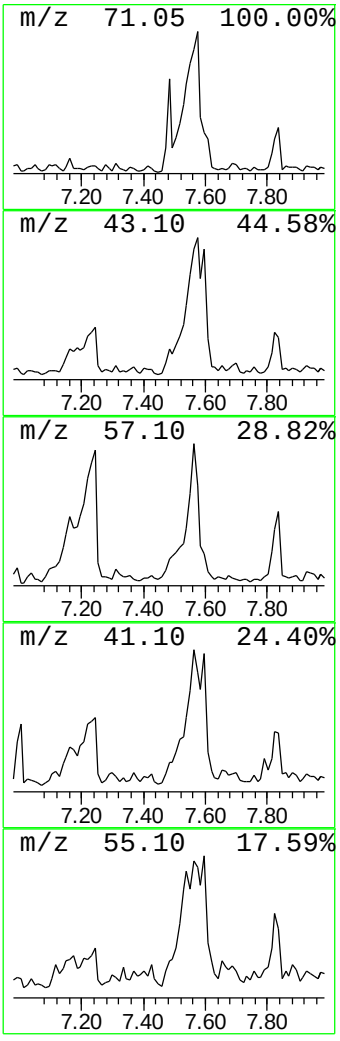
Peak Number 8 Pantolactone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	5.38 ng	253946	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pantolactone	130	C6H10O3	000599-04-2	53
2	Hexanoic acid, 2-tetrahydrofuryl...	200	C11H20O3	002217-34-7	42
3	1,1-Dimethylpropyl 2-ethylhexanoate	214	C13H26O2	1000099-99-2	42
4	3-Cyclopentylpropionic acid, 2-t...	226	C13H22O3	1000293-46-9	40
5	Cyclopentanecarboxylic acid, 2-t...	198	C11H18O3	1000282-42-9	40





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ClientSampleId : MW-5A-012017

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

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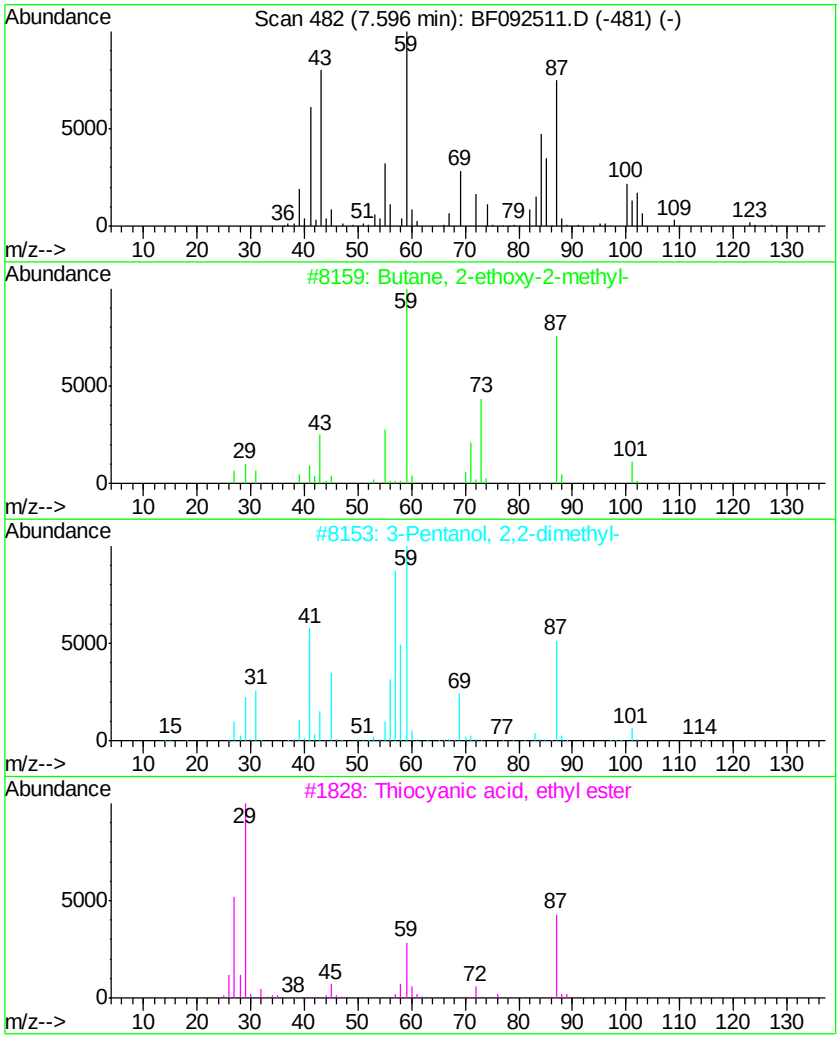
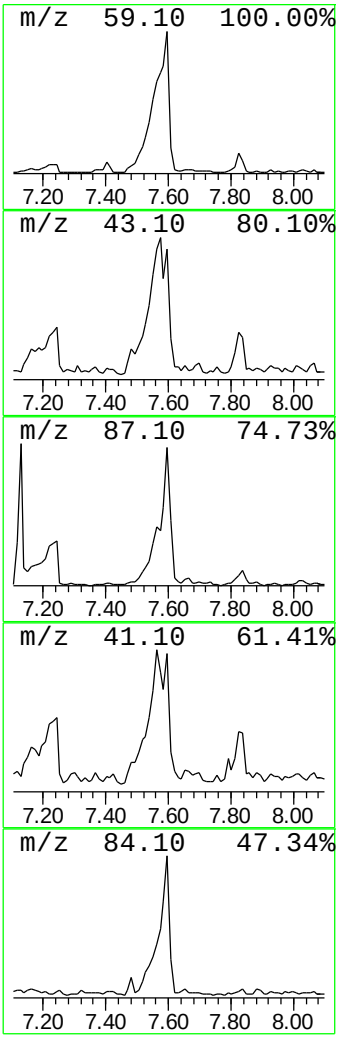
Peak Number 9 Butane, 2-ethoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	14.85 ng	700807	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-ethoxy-2-methyl-	116	C7H16O	000919-94-8	50
2	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	38
3	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	38
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	37
5	Butanoic acid, 4-ethoxy-, methyl...	146	C7H14O3	029006-04-0	37





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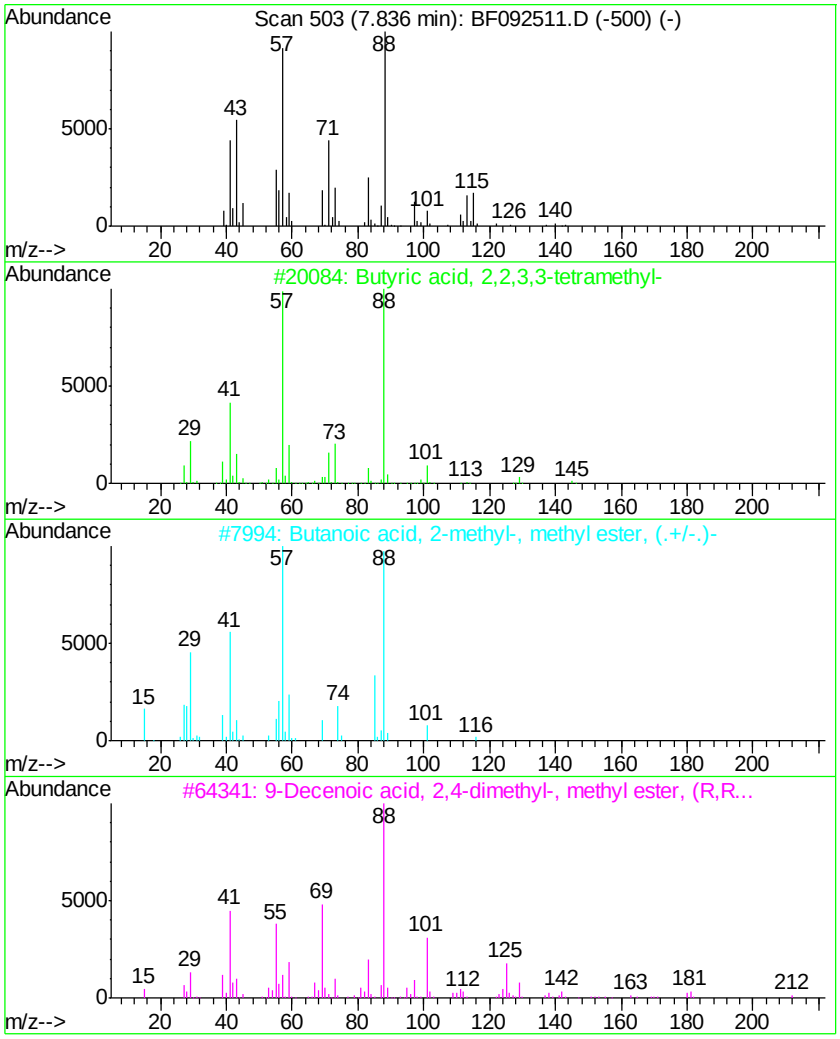
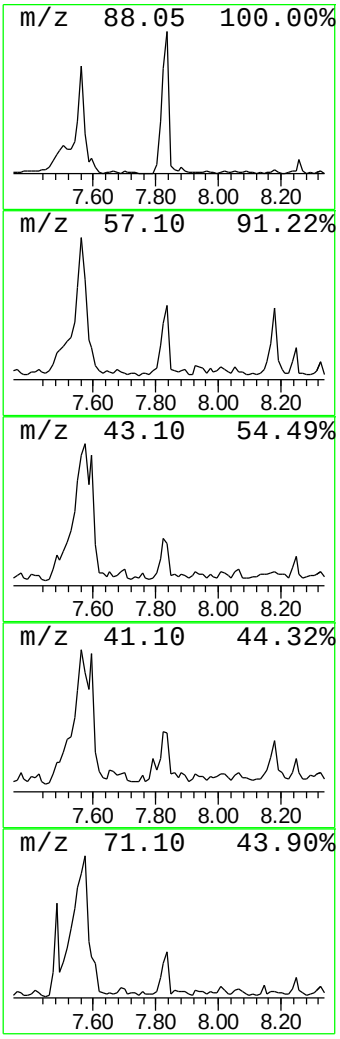
Peak Number 10 Butyric acid, 2,2,3,3-tetra... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.84	9.53 ng	610428	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	50
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	053955-81-0	43
3	9-Decenoic acid, 2,4-dimethyl-, ...	212	C13H24O2	031183-23-0	43
4	Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	38
5	Methyl 2-methyl-3-cyclopropylpro...	142	C8H14O2	062021-35-6	38





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Instrument : BNA_F
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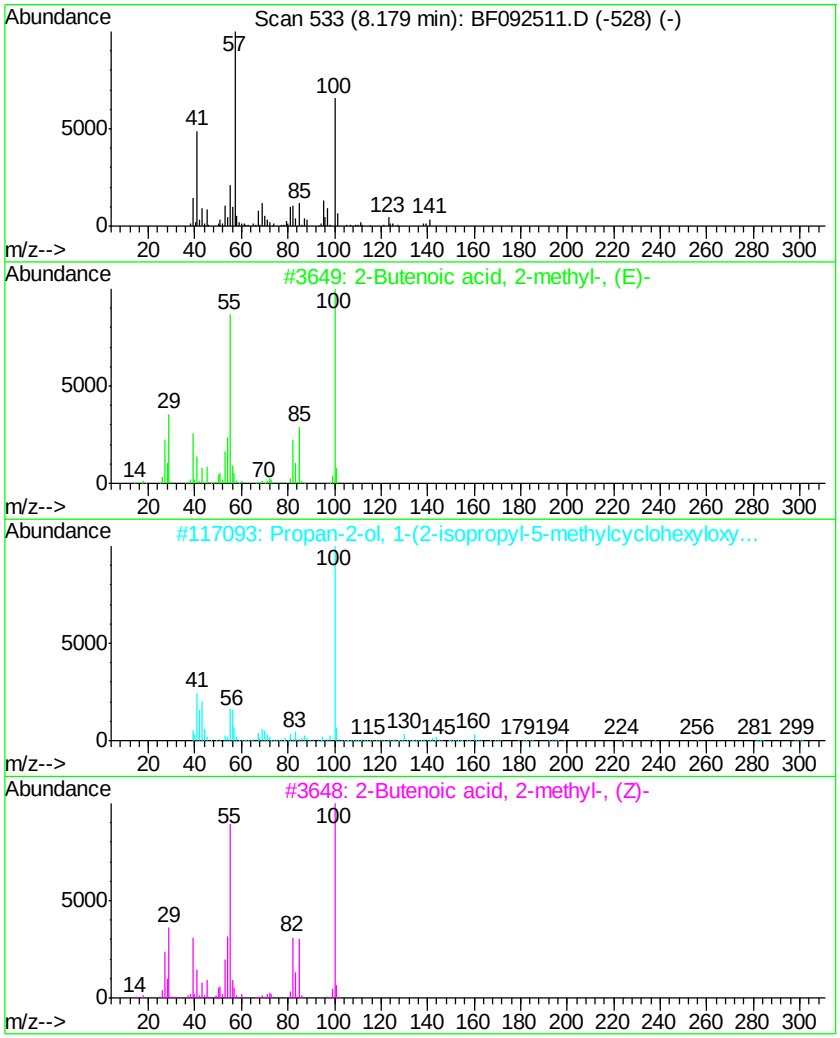
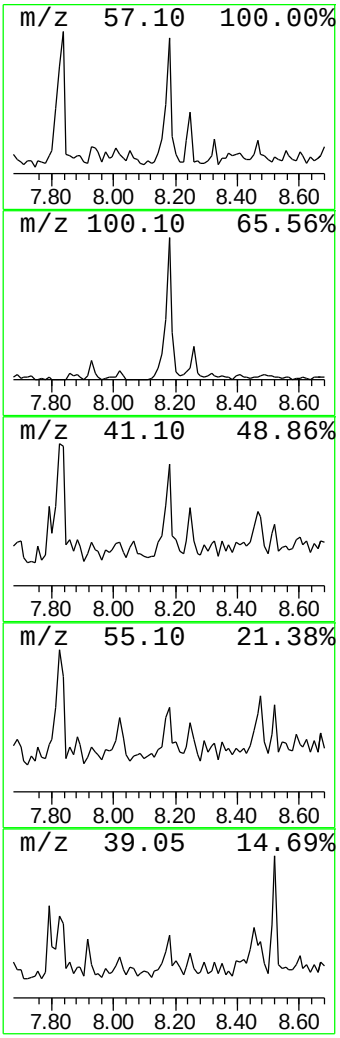
Peak Number 11 unknown8.18 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	4.50 ng	288543	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-methyl-, (E)-	100	C5H8O2	000080-59-1	38
2	Propan-2-ol, 1-(2-isopropyl-5-me...	299	C17H33NO3	320784-52-9	35
3	2-Butenoic acid, 2-methyl-, (Z)-	100	C5H8O2	000565-63-9	35
4	2-Propanone, dimethylhydrazone	100	C5H12N2	013483-31-3	32
5	2-Butenoic acid, 2-methyl-	100	C5H8O2	013201-46-2	27





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ALS Vial : 44 Sample Multiplier: 1

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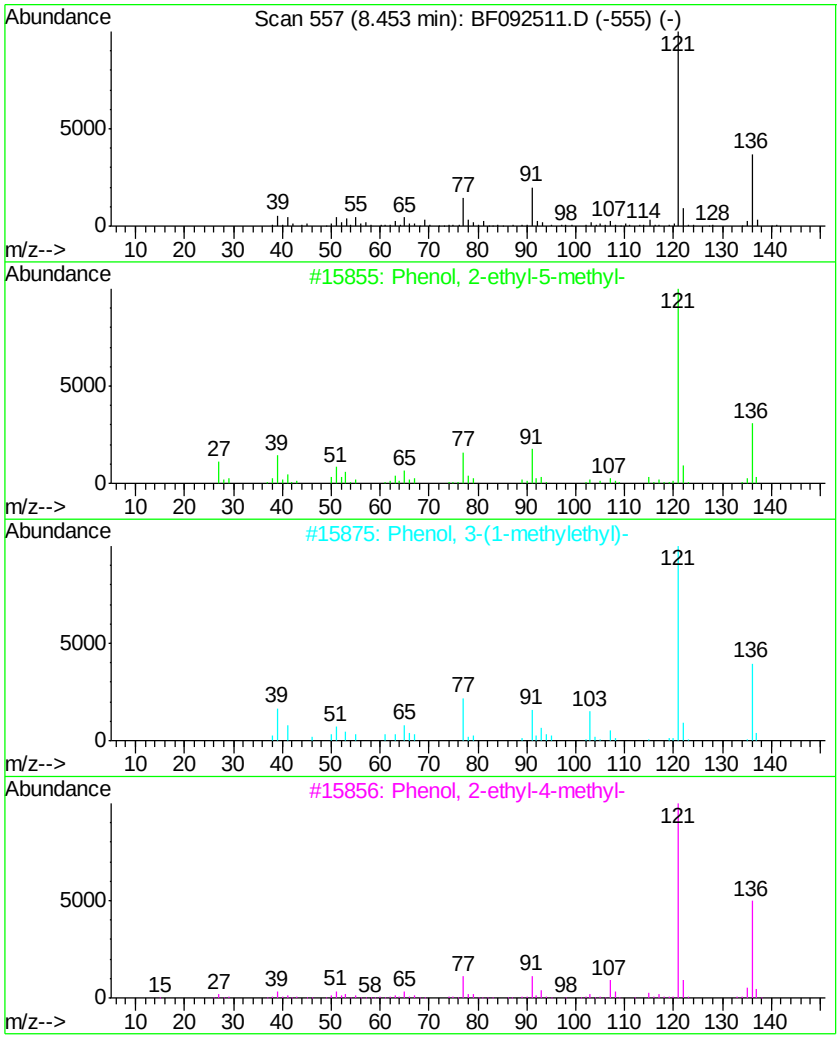
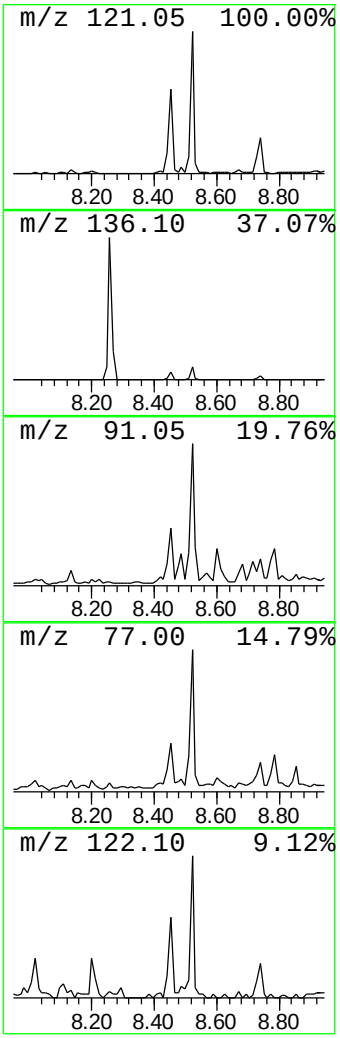
Peak Number 12 Phenol, 2-ethyl-5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	7.60 ng	486972	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-ethyl-5-methyl-	136	C9H12O	001687-61-2	91
2	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	86
3	Phenol, 2-ethyl-4-methyl-	136	C9H12O	003855-26-3	86
4	Benzene, 1-ethyl-4-methoxy-	136	C9H12O	001515-95-3	86
5	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	83





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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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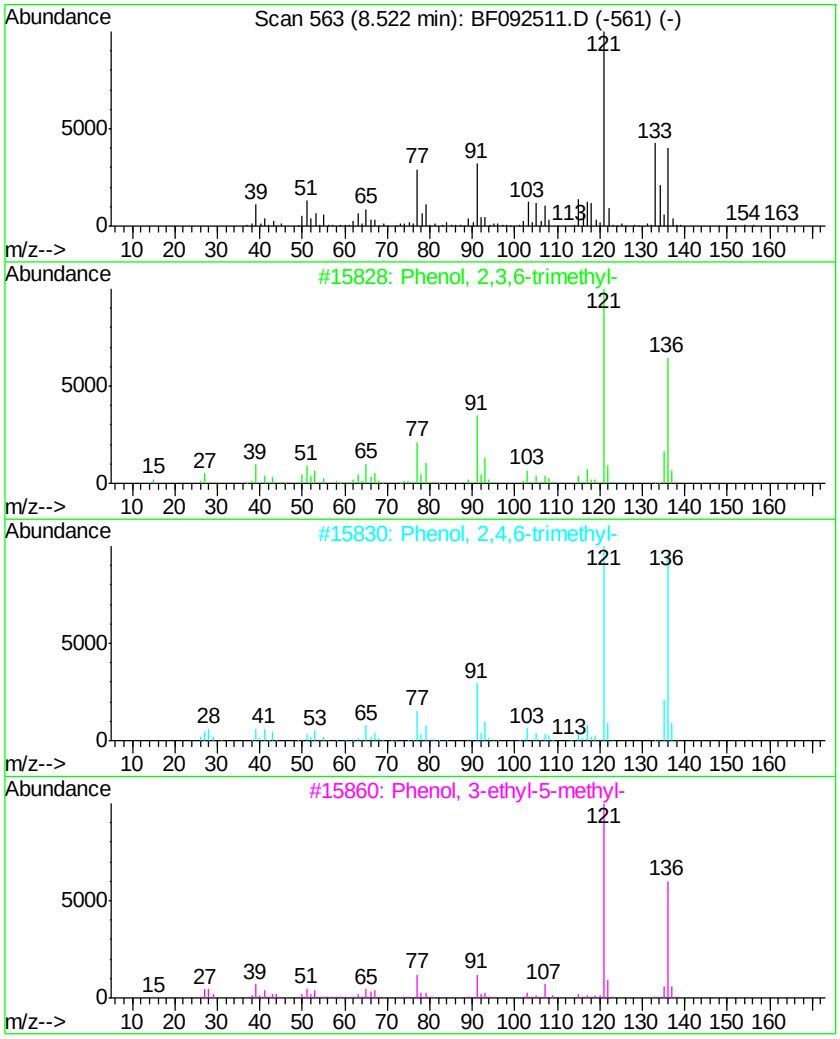
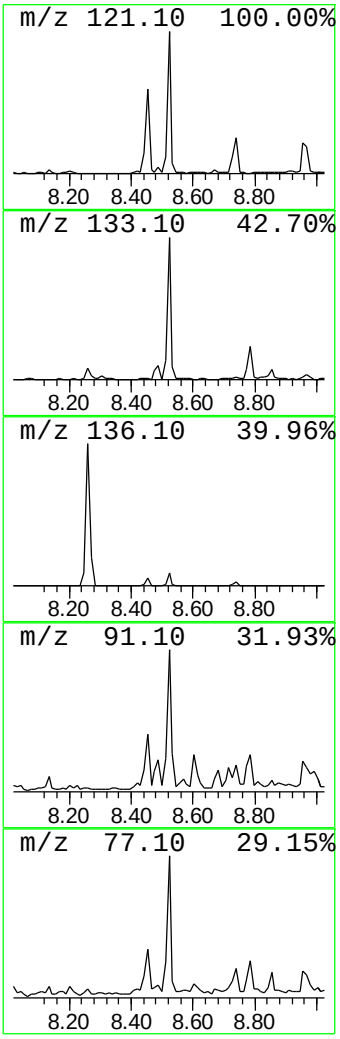
Peak Number 13 Phenol, 2,3,6-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.52	11.64 ng	745781	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,3,6-trimethyl-	136	C9H12O	002416-94-6	62
2	Phenol, 2,4,6-trimethyl-	136	C9H12O	000527-60-6	62
3	Phenol, 3-ethyl-5-methyl-	136	C9H12O	000698-71-5	58
4	Hydrazine, 1-(4-ethylphenyl)-	136	C8H12N2	054840-34-5	49
5	Phenol, 2-ethyl-4-methyl-	136	C9H12O	003855-26-3	49





Library Search Compound Report

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Sample : I1398-08
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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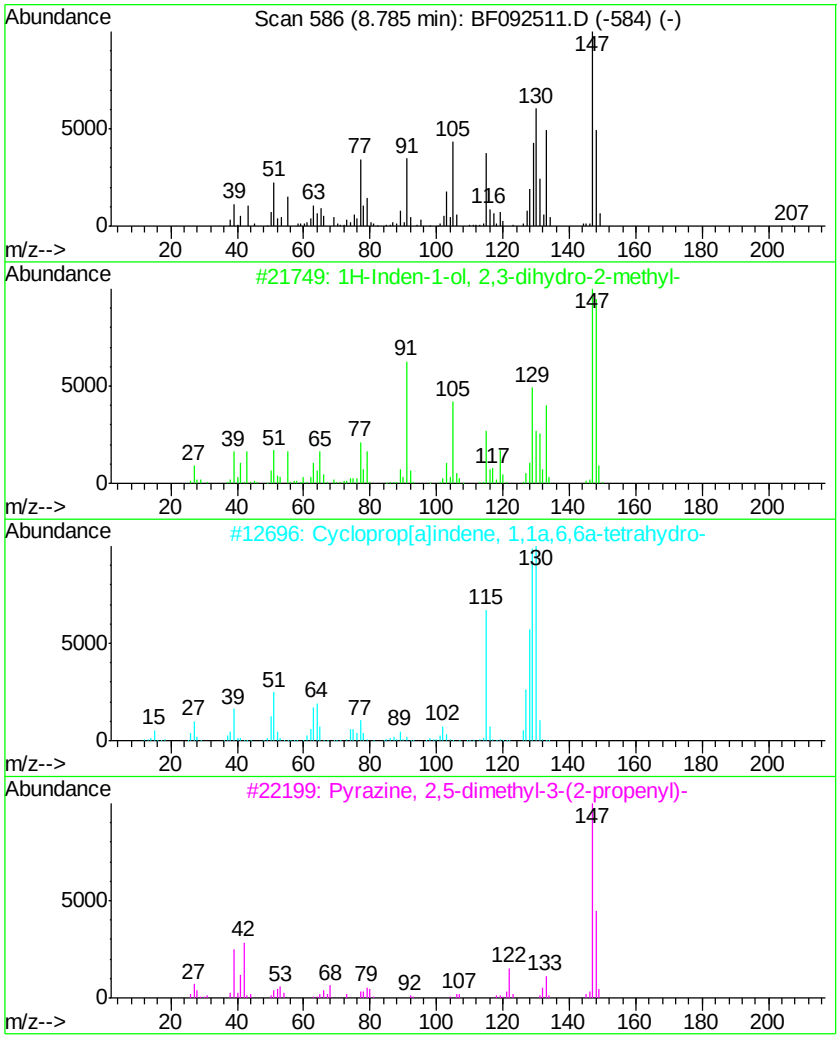
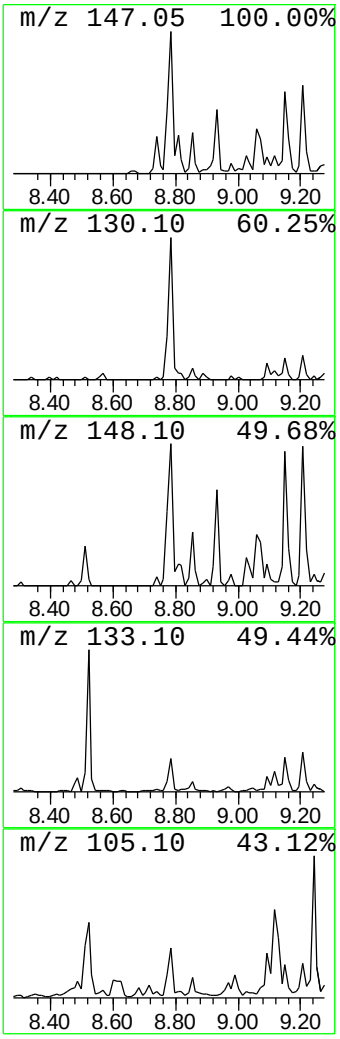
Peak Number 14 unknown8.78 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.78	3.81 ng	244441	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-ol, 2,3-dihydro-2-met...	148	C10H12O	017496-18-3	35
2	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	30
3	Pyrazine, 2,5-dimethyl-3-(2-prop...	148	C9H12N2	055138-69-7	27
4	Pyrazine, 3,5-dimethyl-2-(2-prop...	148	C9H12N2	055138-70-0	27
5	2-Methylindene	130	C10H10	002177-47-1	25





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TIC Library : C:\DATABASE\NIST02.L
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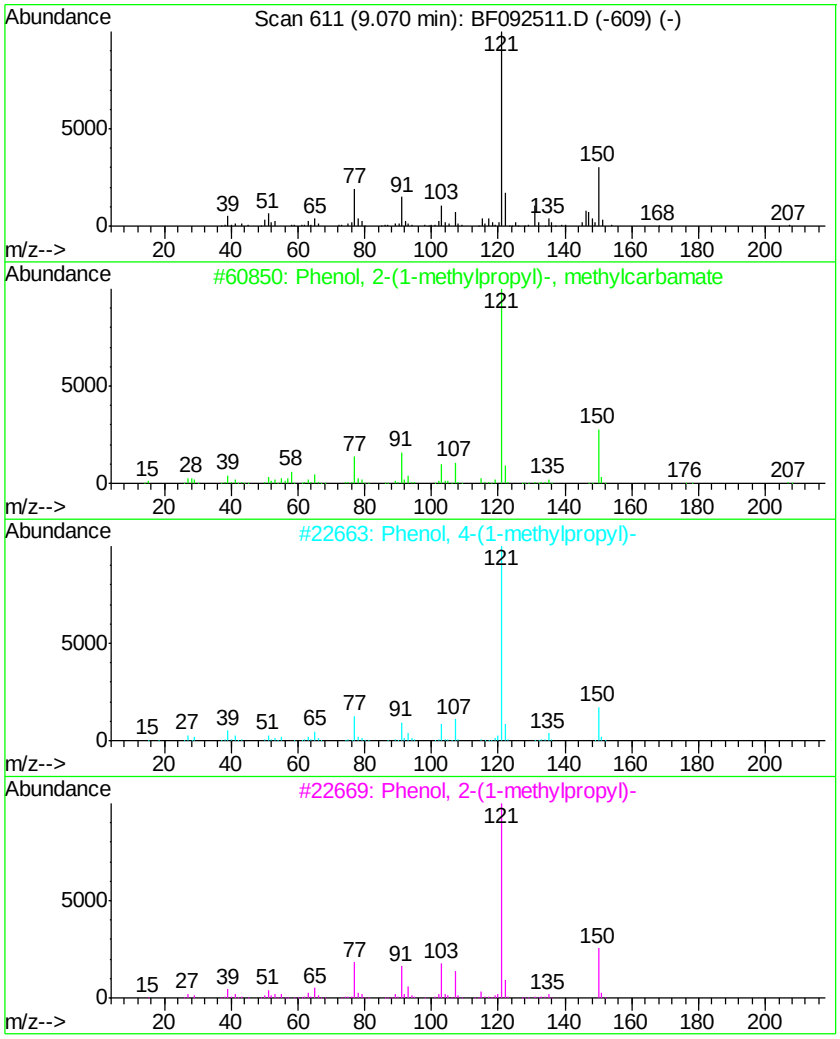
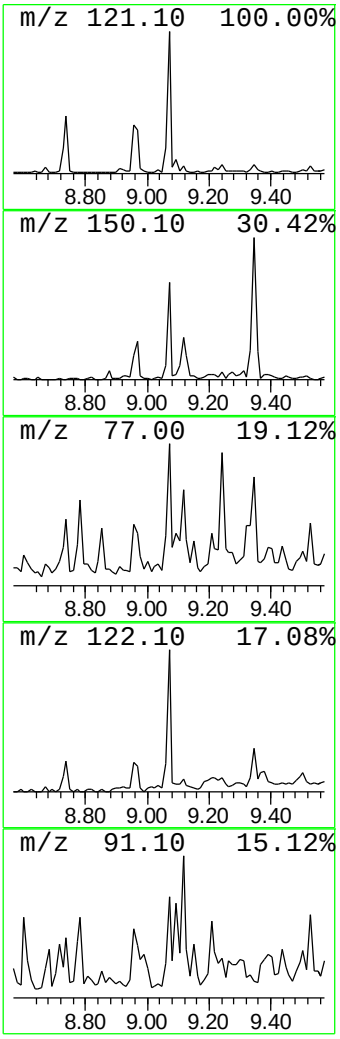
Peak Number 15 Phenol, 2-(1-methylpropyl)-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.07	4.80 ng	307675	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1-methylpropyl)-, met...	207	C12H17NO2	003766-81-2	76
2	Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	72
3	Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	64
4	Phenol, 2-ethyl-5-methyl-	136	C9H12O	001687-61-2	53
5	p-Sec-butylphenyl acetate	192	C12H16O2	003245-24-7	53





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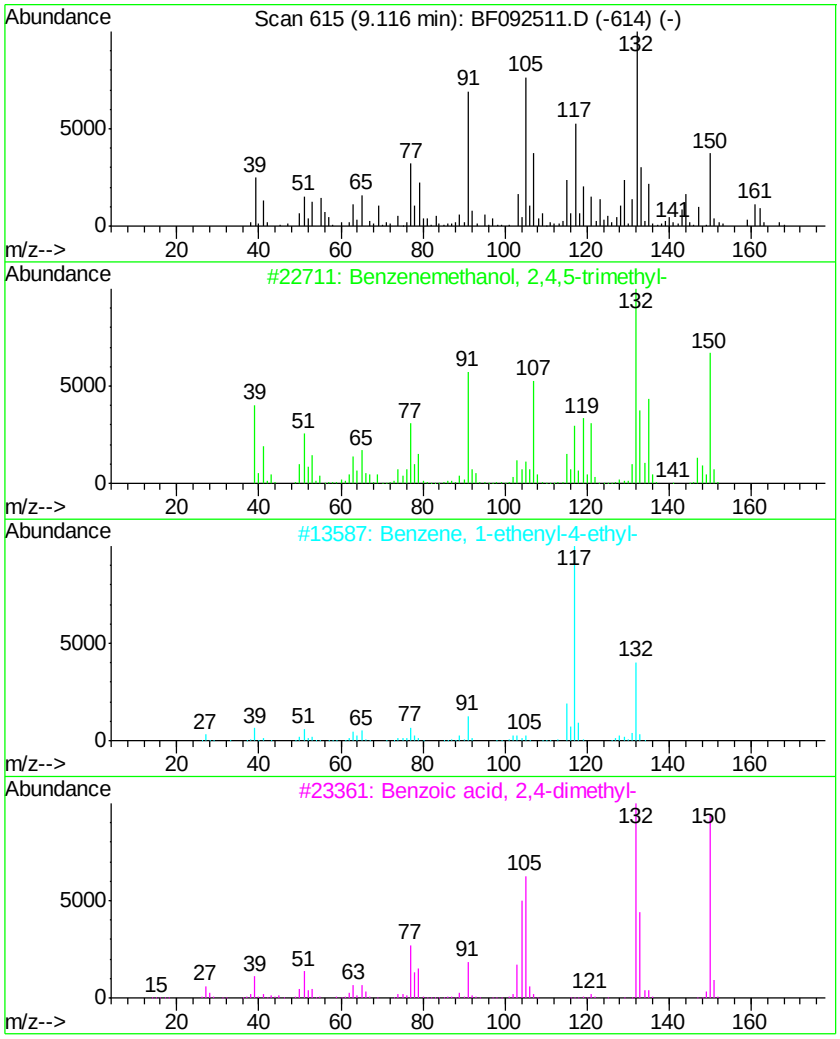
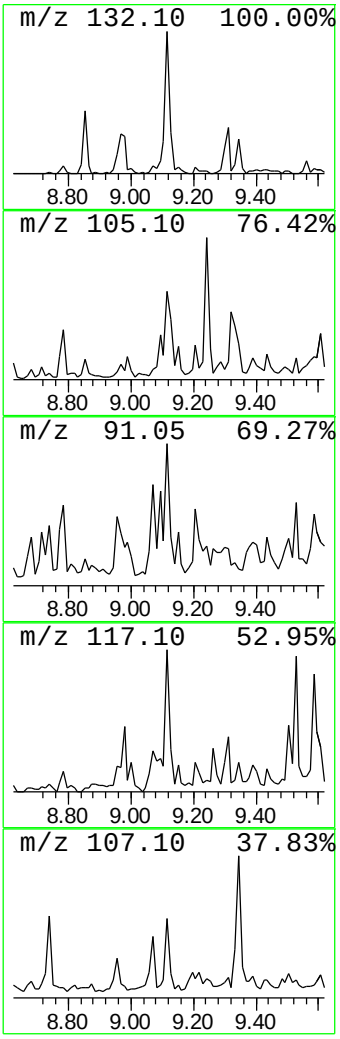
Peak Number 16 unknown9.12 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.12	4.88 ng	312951	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, 2,4,5-trimethyl-	150	C10H14O	004393-05-9	43
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	43
3	Benzoic acid, 2,4-dimethyl-	150	C9H10O2	000611-01-8	41
4	Benzeneethanol, .alpha.,.alpha.-...	192	C12H16O2	000151-05-3	38
5	1,1-Cyclopropanedicarbonitrile, ...	210	C14H14N2	074764-41-3	38





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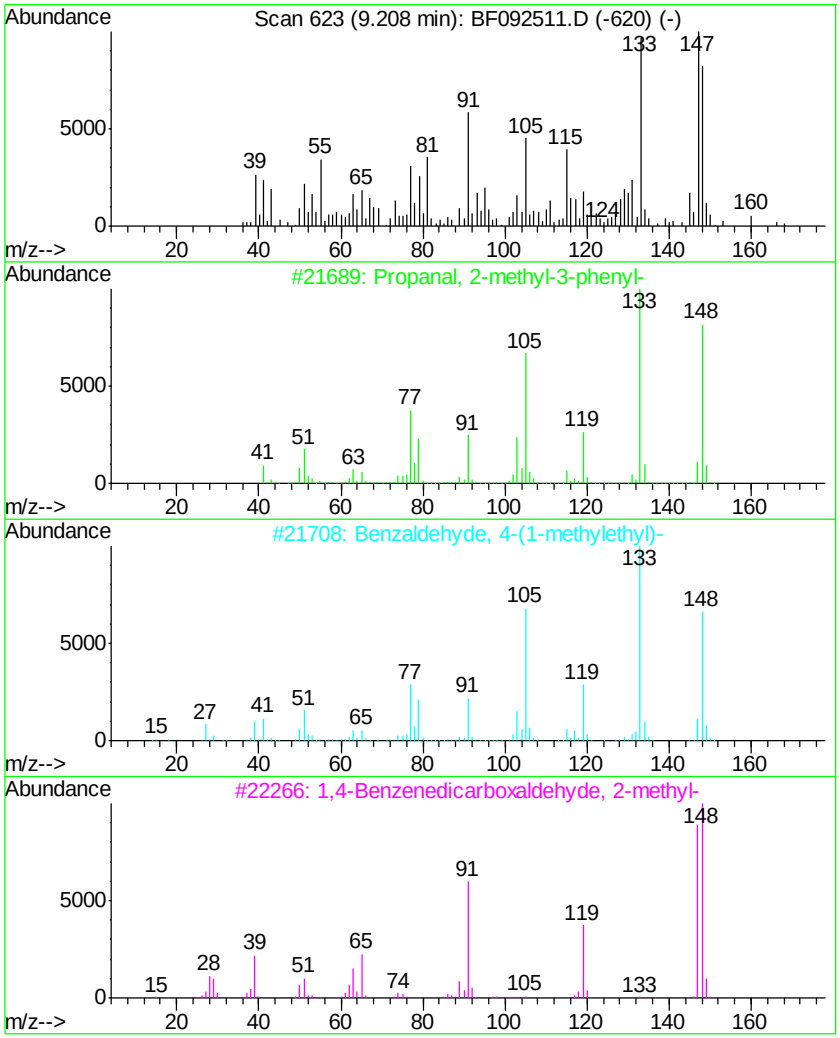
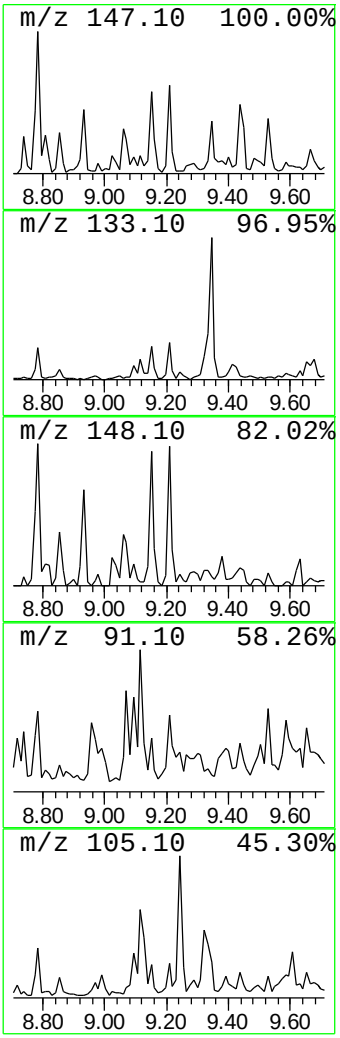
Peak Number 17 Propanal, 2-methyl-3-phenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.21	5.70 ng	375741	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-3-phenyl-	148	C10H12O	1000131-87-6	89
2	Benzaldehyde, 4-(1-methylethyl)-	148	C10H12O	000122-03-2	86
3	1,4-Benzenedicarboxaldehyde, 2-m...	148	C9H8O2	027587-17-3	62
4	2-Isopropenyl-3,6-dimethylpyrazine	148	C9H12N2	1000109-60-7	62
5	2-Propenoic acid, 3-phenyl-	148	C9H8O2	000621-82-9	49





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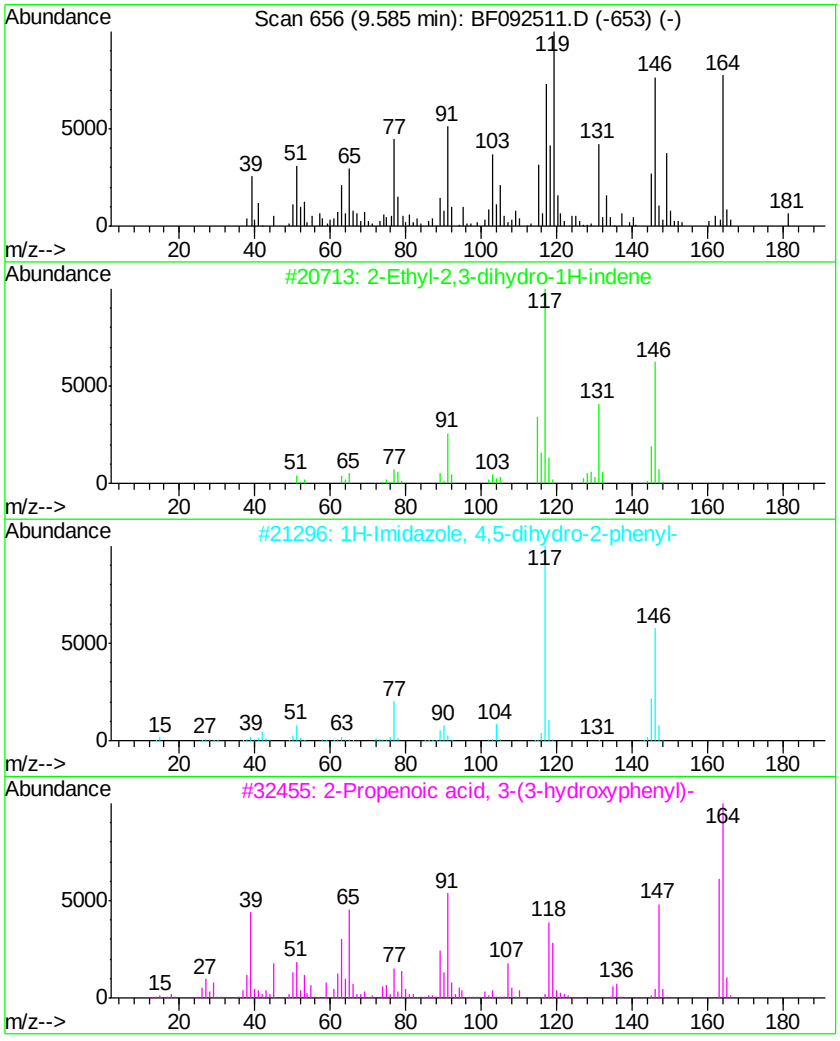
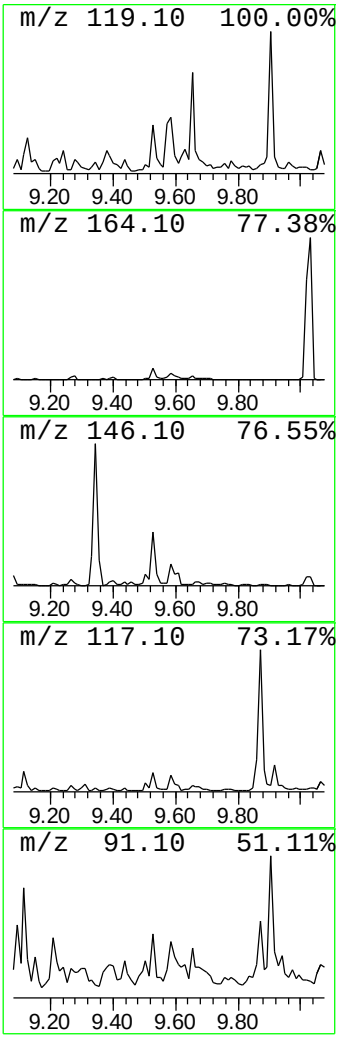
Peak Number 18 unknown9.58 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.58	4.22 ng	277841	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-2,3-dihydro-1H-indene	146	C11H14	056147-63-8	46
2	1H-Imidazole, 4,5-dihydro-2-phenyl-	146	C9H10N2	000936-49-2	46
3	2-Propenoic acid, 3-(3-hydroxyph...	164	C9H8O3	000588-30-7	44
4	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	38
5	Phenol, 2-methoxy-5-(1-propenyl)...	164	C10H12O2	019784-98-6	35





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Data File : BF092511.D
Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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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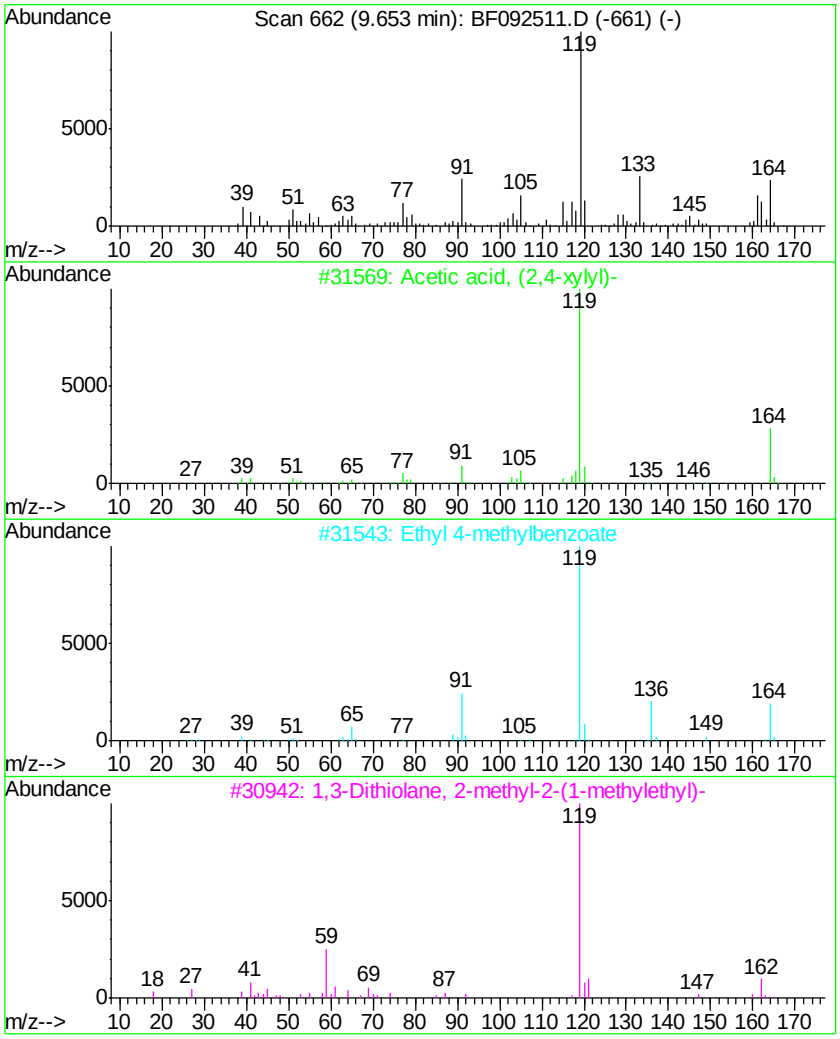
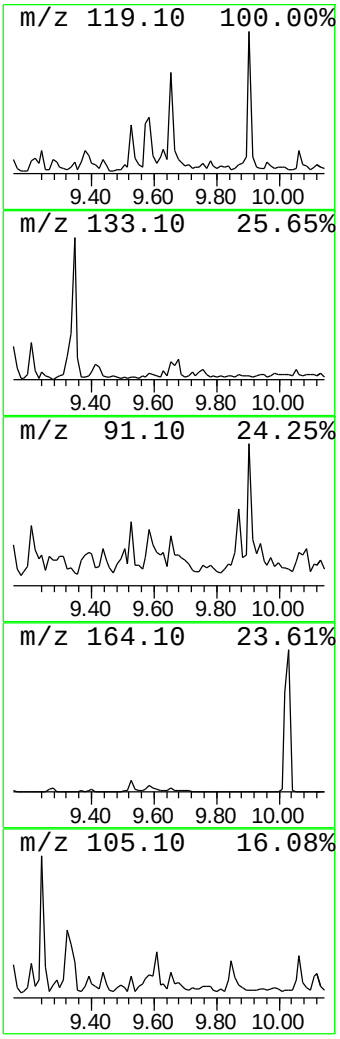
Peak Number 19 Acetic acid, (2,4-xylyl)- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.65	4.12 ng	271616	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	52
2	Ethyl 4-methylbenzoate	164	C10H12O2	000094-08-6	49
3	1,3-Dithiolane, 2-methyl-2-(1-me...	162	C7H14S2	006008-88-4	49
4	Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	49
5	Benzene, 1-methyl-4-(1-methyleth...	134	C10H14	000099-87-6	49





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012617\
Data File : BF092511.D
Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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

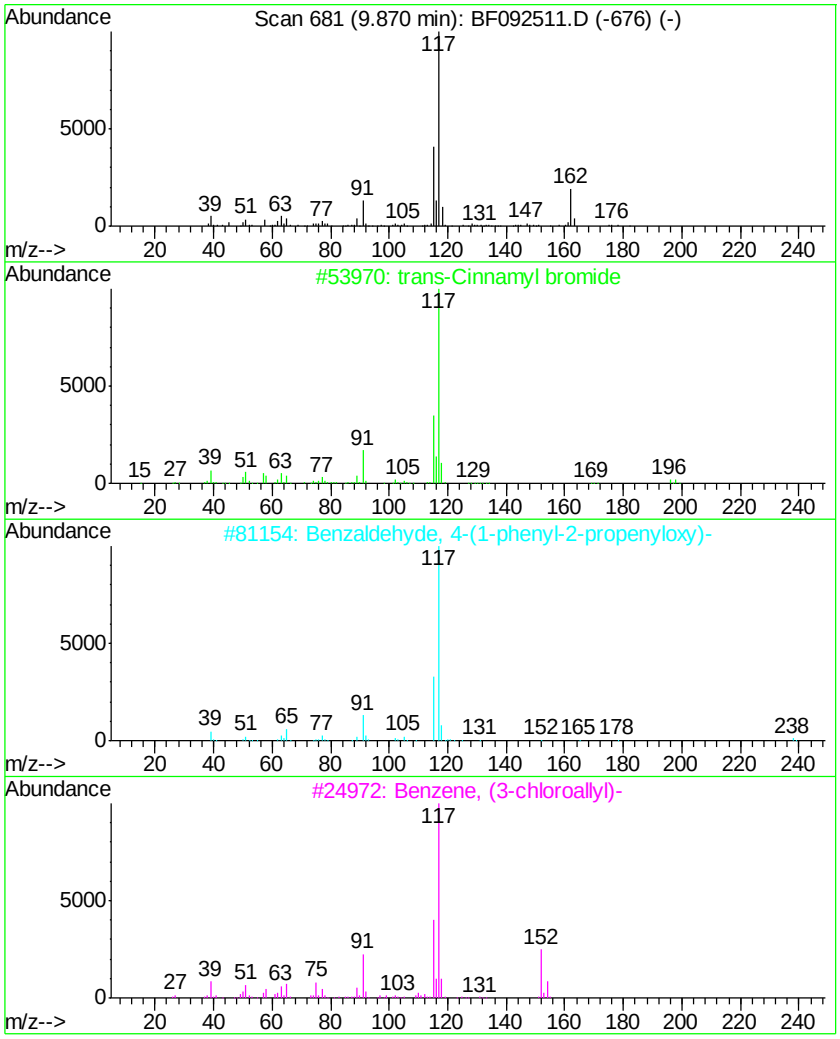
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

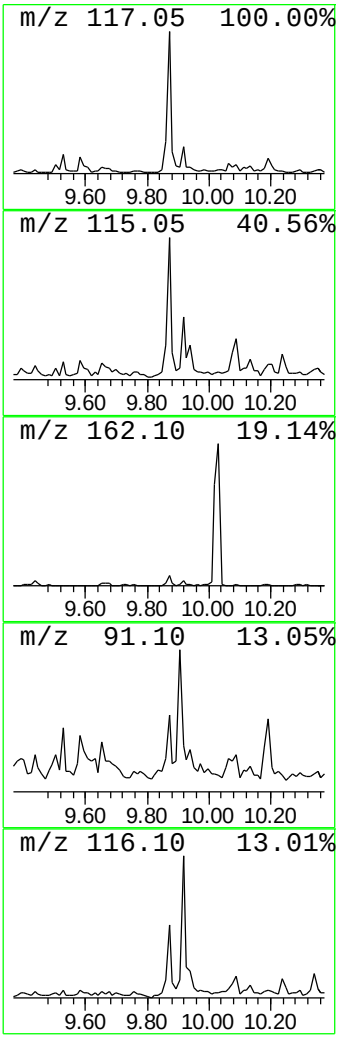
****

Peak Number 20 trans-Cinnamyl bromide Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	4.74 ng	312739	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	64
2	Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	59
3	Benzene, (3-chloroallyl)-	152	C9H9Cl	006268-37-7	59
4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	59
5	Benzene, (chloromethyl)ethenyl-	152	C9H9Cl	030030-25-2	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012617\
Data File : BF092511.D
Acq On : 26 Jan 2017 8:35
Operator : SJ/MA
Sample : I1398-08
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-012017

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
2-Butanol, 2,3-di...	3.18	4.6	ng	218413	1	6.97	943985	20.0
2-Pentanone, 4-hy...	5.15	13.4	ng	630080	1	6.97	943985	20.0
Cyclopentanol, 3-...	5.21	3.8	ng	177073	1	6.97	943985	20.0
unknown6.73	6.73	73.5	ng	3468840	1	6.97	943985	20.0
unknown7.16	7.16	7.4	ng	348181	1	6.97	943985	20.0
Hexanoic acid, 2,...	7.24	21.1	ng	994225	1	6.97	943985	20.0
Pantolactone	7.48	5.4	ng	253946	1	6.97	943985	20.0
Butane, 2-ethoxy-...	7.60	14.9	ng	700807	1	6.97	943985	20.0
Butyric acid, 2,2...	7.84	9.5	ng	610428	2	8.26	1281710	20.0
unknown8.18	8.18	4.5	ng	288543	2	8.26	1281710	20.0
Phenol, 2-ethyl-5...	8.45	7.6	ng	486972	2	8.26	1281710	20.0
Phenol, 2,3,6-tri...	8.52	11.6	ng	745781	2	8.26	1281710	20.0
unknown8.78	8.78	3.8	ng	244441	2	8.26	1281710	20.0
Phenol, 2-(1-meth...	9.07	4.8	ng	307675	2	8.26	1281710	20.0
unknown9.12	9.12	4.9	ng	312951	2	8.26	1281710	20.0
Propanal, 2-methy...	9.21	5.7	ng	375741	3	10.03	1318190	20.0
unknown9.58	9.58	4.2	ng	277841	3	10.03	1318190	20.0
Acetic acid, (2,4...	9.65	4.1	ng	271616	3	10.03	1318190	20.0
trans-Cinnamyl br...	9.87	4.7	ng	312739	3	10.03	1318190	20.0