LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092944.D
Acq On : 14 Feb 2017 15:20
Operator : SJ/MA
Sample : I1794-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 22A-9-11

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-BF013017.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	3.813	148	151	158	rBV	33539	52569	1.16%	0.141%
2	5.047	257	259	263	rBV	451495	565228	12.46%	1.516%
3	5.321	281	283	286	rBV	116265	107717	2.37%	0.289%
4	5.436	290	293	295	rBV	261786	420605	9.27%	1.128%
5	5.470	295	296	299	rVB	1702354	1657059	36.52%	4.443%
6	5.607	306	308	311	rVB	54477	50516	1.11%	0.135%
7	5.699	314	316	318	rBV2	138561	138428	3.05%	0.371%
8	6.396	374	377	378	rBV	90726	87255	1.92%	0.234%
9	6.419	378	379	381	rVV	40470	50213	1.11%	0.135%
10	6.464	381	383	385	rVV	57379	70606	1.56%	0.189%
11	6.510	385	387	389	rVV	1000200	1163507	25.64%	3.120%
12	6.556	389	391	393	rVV	58461	54609	1.20%	0.146%
13	6.636	396	398	401	rVV	2298370	3152623	69.47%	8.454%
14	6.693	401	403	406	rVB	338403	290104	6.39%	0.778%
15	6.876	417	419	421	rBV	924107	945009	20.82%	2.534%
16	6.933	421	424	427	rVB	118479	137689	3.03%	0.369%
17	7.024	430	432	435	rBV	2153445	2960114	65.23%	7.937%
18	7.196	445	447	449	rBV	94467	89739	1.98%	0.241%
19	7.264	451	453	457	rVB2	31818	53464	1.18%	0.143%
20	7.344	457	460	461	rBV	37024	50379	1.11%	0.135%
21	7.436	464	468	471	rBV	1995959	2627699	57.90%	7.046%
22	7.642	483	486	487	rBV2	48338	61999	1.37%	0.166%
23	7.676	487	489	491	rVB	77109	78655	1.73%	0.211%
24	7.836	500	503	505	rVB2	46390	84262	1.86%	0.226%
25	7.893	505	508	510	rBV2	149470	181586	4.00%	0.487%
26	8.179	529	533	536	rVV	1851956	3001735	66.15%	8.049%
27	8.236	536	538	541	rVB2	74166	97837	2.16%	0.262%
28	8.876	591	594	596	rVB	397954	502634	11.08%	1.348%
29	8.967	600	602	604	rBV	327385	313733	6.91%	0.841%
30	9.082	609	612	617	rBV3	33209	57406	1.27%	0.154%
31	9.242	623	626	628	rBV	3399783	4537993	100.00%	12.168%
32	9.333	633	634	637	rVB	98968	78817	1.74%	0.211%
33	9.436	640	643	645	rVB	36107	61985	1.37%	0.166%
34	9.493	645	648	651	rBV	91243	134410	2.96%	0.360%

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Integrator: RTE
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.573	653	655	656	rBV	144371	159951	3.52%	0.429%
36	9.596	656	657	659	rVV	86936	75534	1.66%	0.203%
37	9.687	661	665	670	rBV	68663	98871	2.18%	0.265%
38	9.767	670	672	674	rBV2	47202	60101	1.32%	0.161%
39	9.916	682	685	686	rBV	1410327	1519921	33.49%	4.076%
40	9.939	686	687	690	rVB	200410	233436	5.14%	0.626%
41	10.122	700	703	705	rBV2	125048	222174	4.90%	0.596%
42	10.328	717	721	725	rBV3	54471	109926	2.42%	0.295%
43	10.430	725	730	731	rBV3	39755	64453	1.42%	0.173%
44	10.453	731	732	735	rVB	158765	177375	3.91%	0.476%
45	10.522	735	738	745	rBV3	35244	72344	1.59%	0.194%
46	10.705	751	754	756	rBV	2368744	2552557	56.25%	6.845%
47	10.819	762	764	768	rVB2	34991	64722	1.43%	0.174%
48	11.390	812	814	818	rBV2	1252450	1671045	36.82%	4.481%
49	12.979	950	953	956	rBV	3647066	3874541	85.38%	10.389%
50	13.894	1029	1033	1036	rBV2	25446	49468	1.09%	0.133%
51	14.031	1042	1045	1047	rBV	1368591	1357395	29.91%	3.640%
52	15.459	1167	1170	1173	rBV	741738	1011248	22.28%	2.712%

Sum of corrected areas: 37293246

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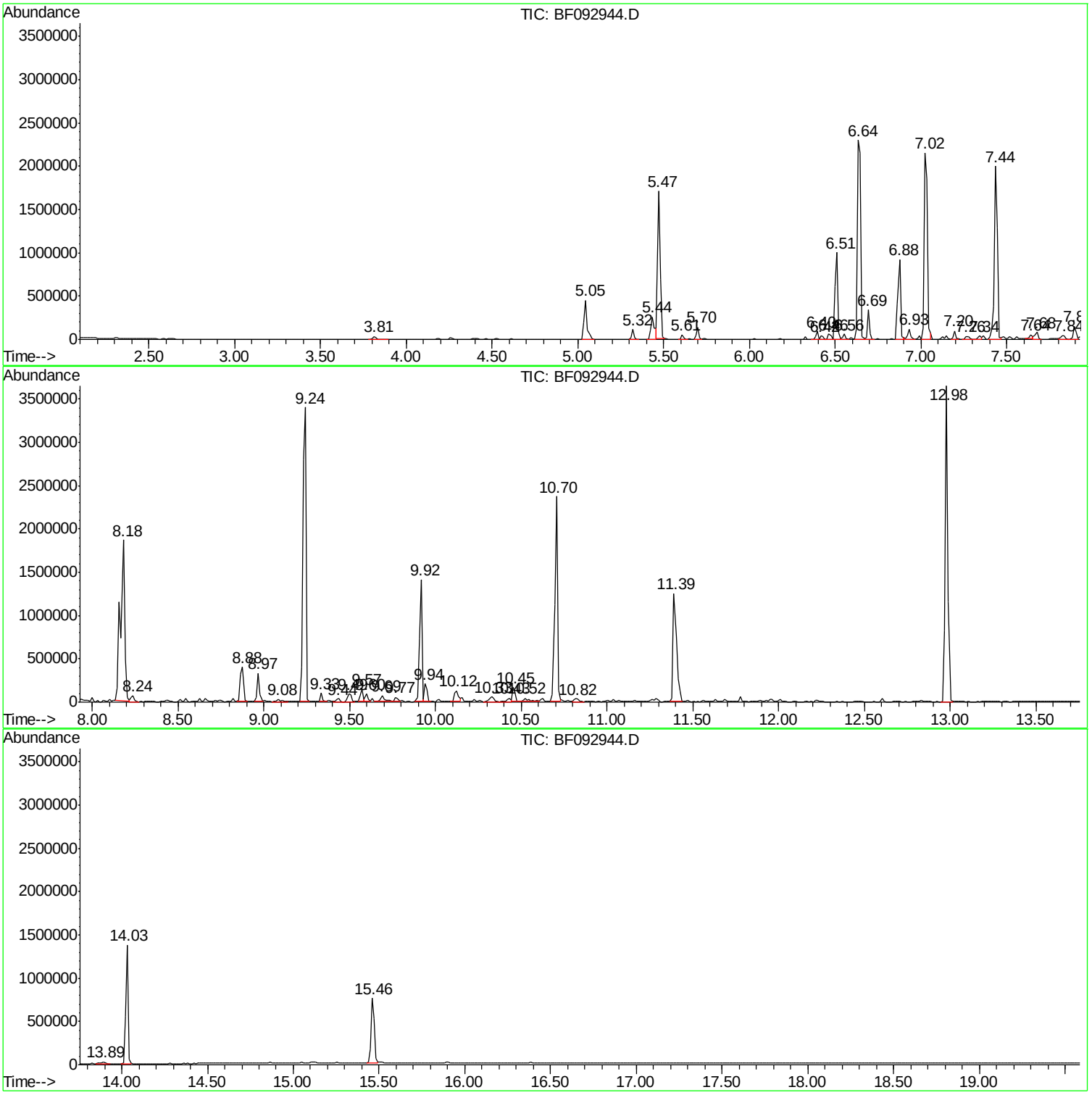
Instrument :
BNA_F
ClientSampleId :
22A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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Sample : I1794-06
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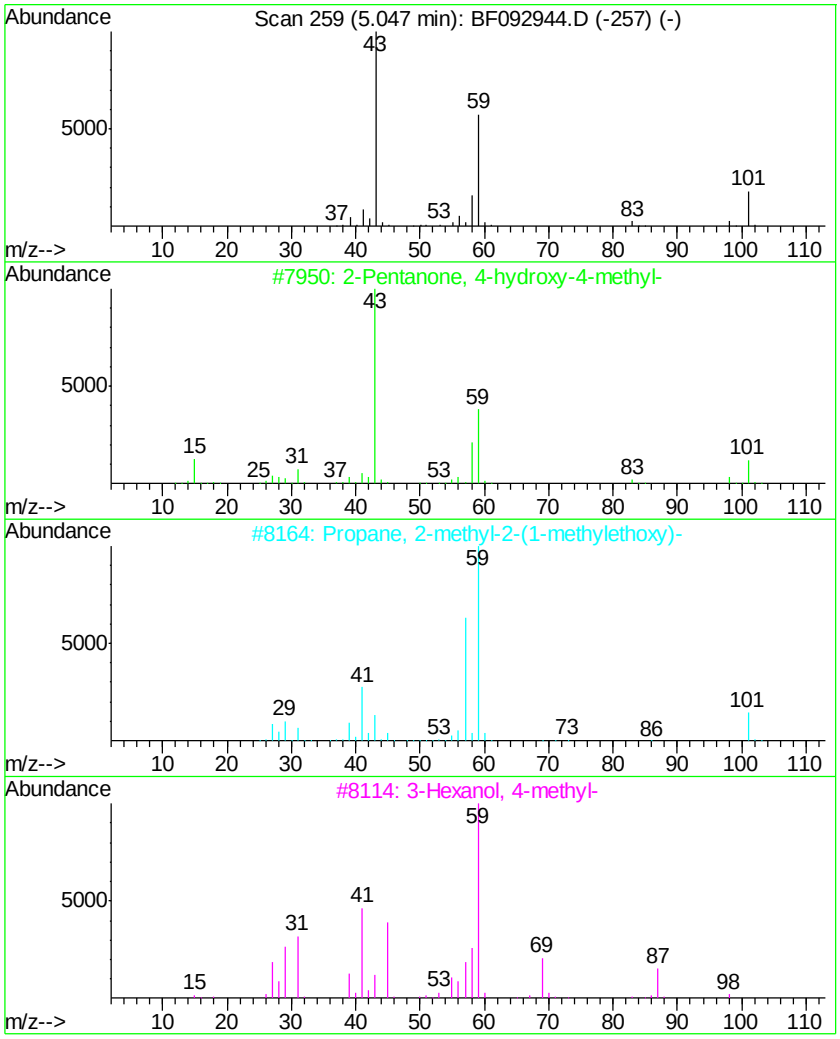
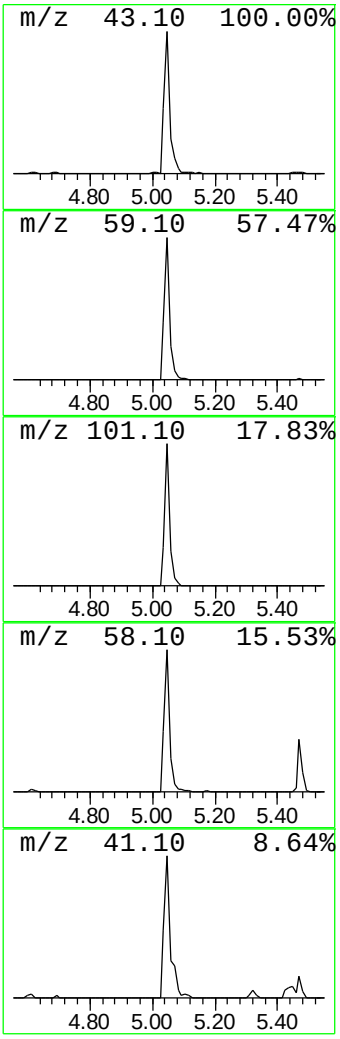
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	11.96 ng	565228	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092944.D
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Operator : SJ/MA
Sample : I1794-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 22A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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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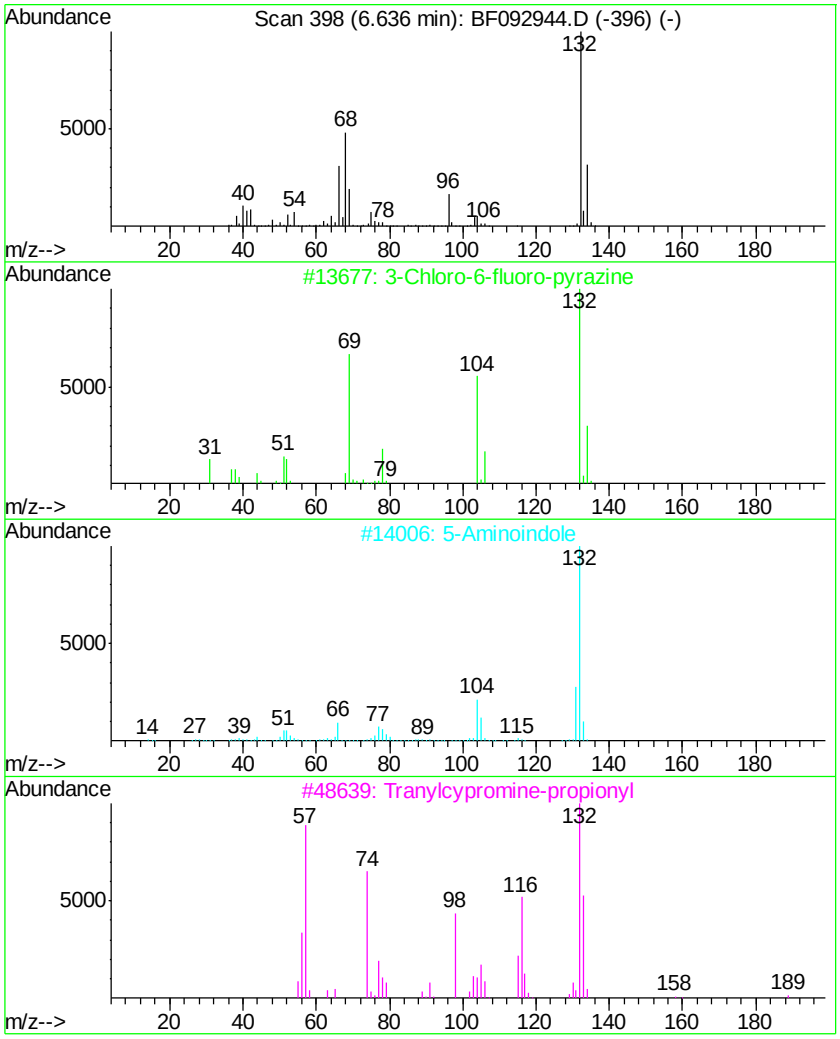
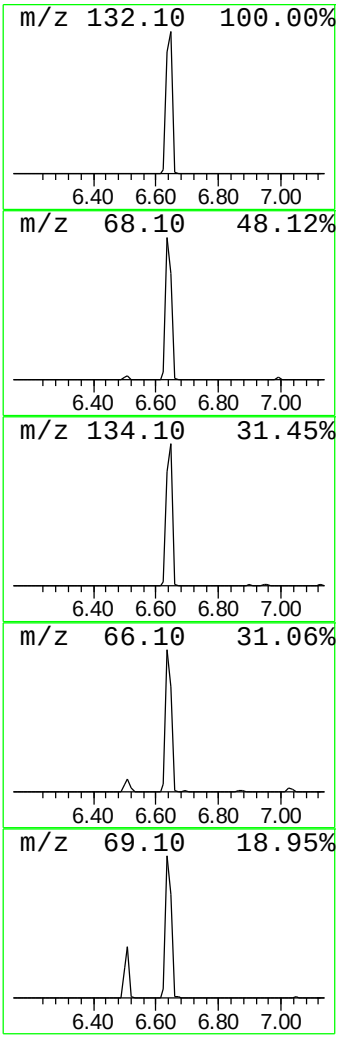
Peak Number 4 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	66.72 ng	3152620	1,4-Dichlorobenzene-d4	6.88

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	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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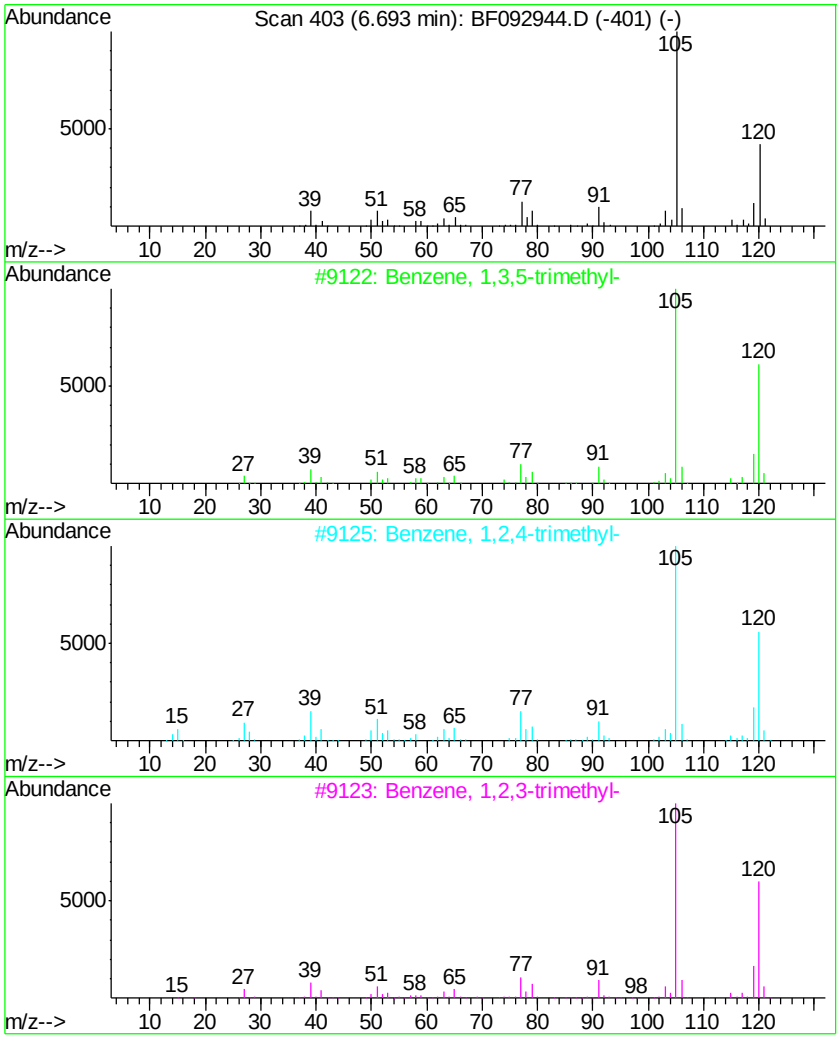
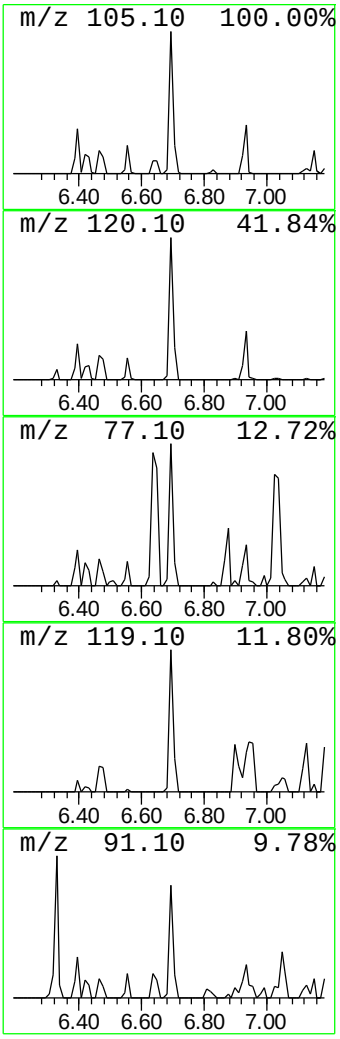
Peak Number 5 Benzene, 1,3,5-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	6.14 ng	290104	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	97
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





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Misc :
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Instrument : BNA_F
ClientSampleId : 22A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
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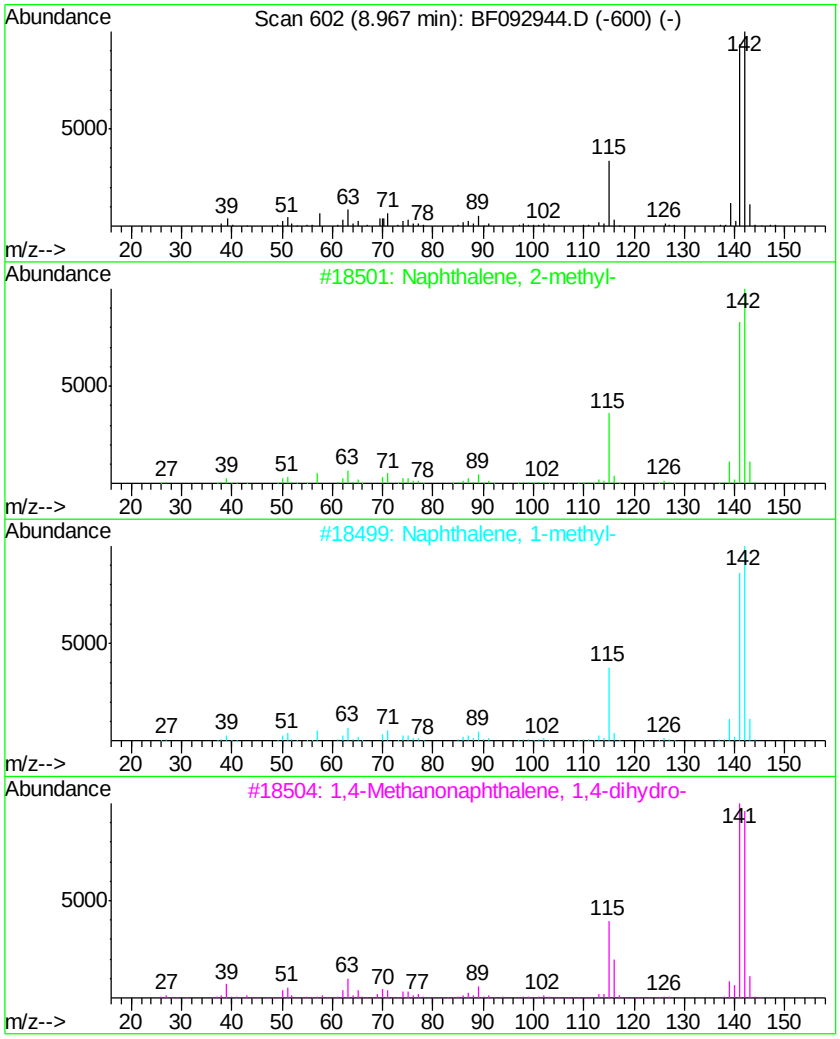
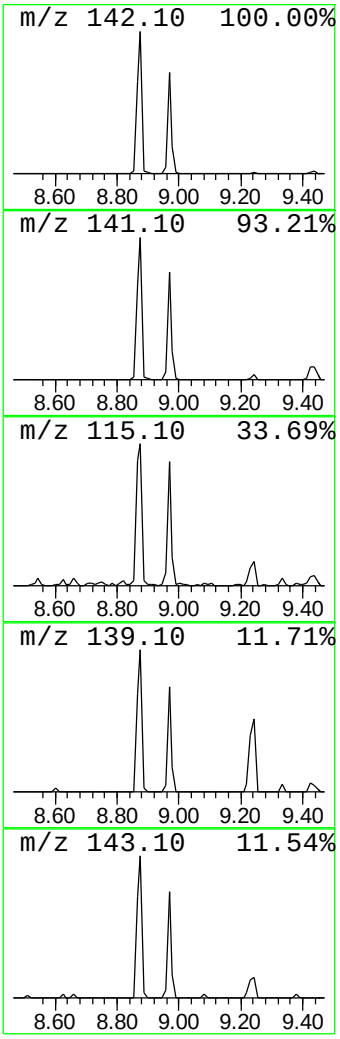
Peak Number 8 Naphthalene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.97	2.09 ng	313733	Naphthalene-d8	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	47





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Misc :
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Instrument : BNA_F
ClientSampleId : 22A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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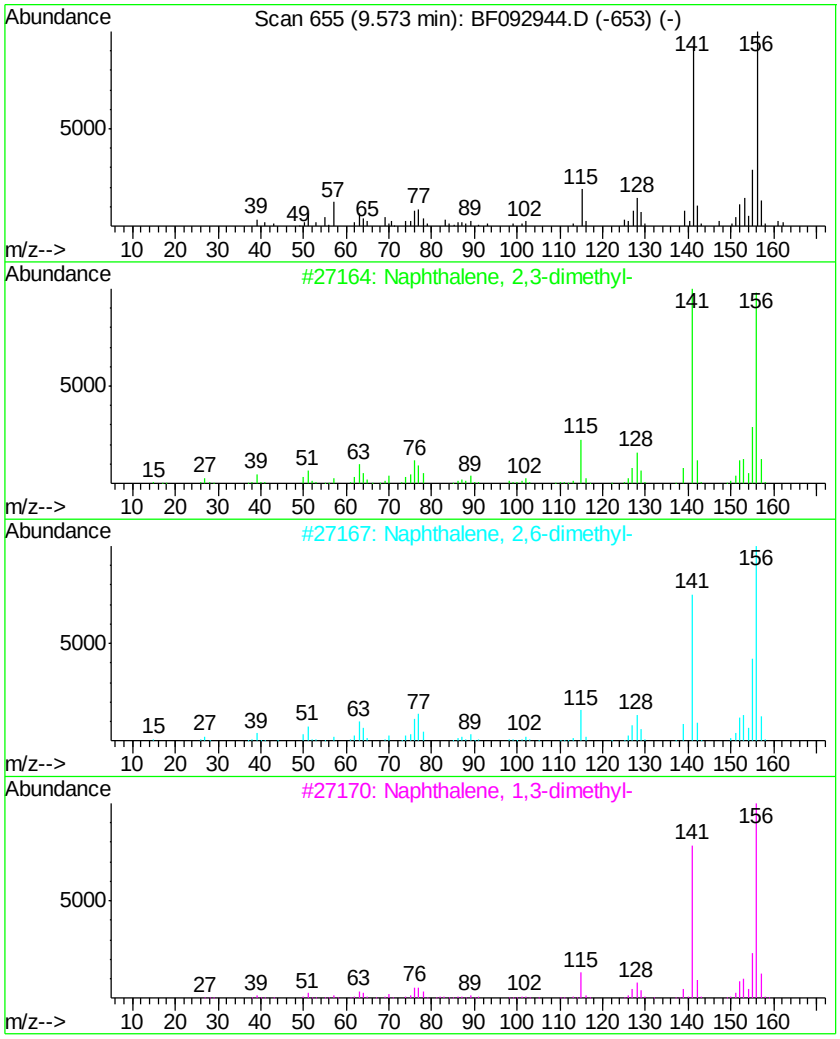
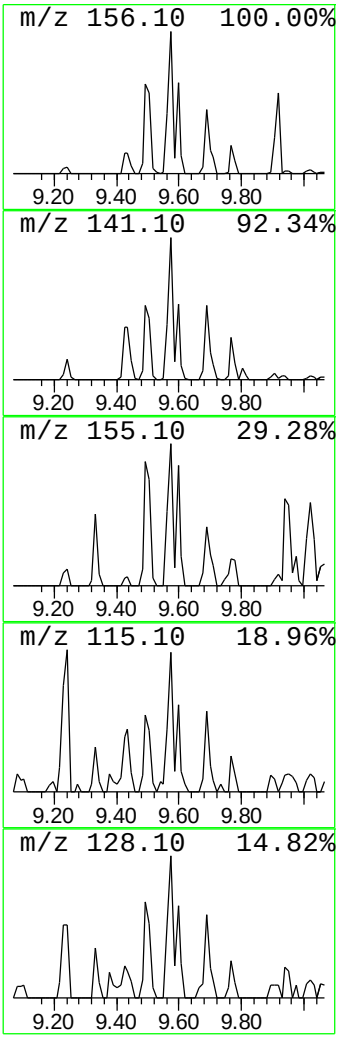
Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	2.10 ng	159951	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	12.0	ng	565228	1	6.88	945009	20.0
unknown6.64	6.64	66.7	ng	3152620	1	6.88	945009	20.0
Benzene, 1,3,5-tr...	6.69	6.1	ng	290104	1	6.88	945009	20.0
Naphthalene, 1-me...	8.97	2.1	ng	313733	2	8.16	3001740	20.0
Naphthalene, 2,3-...	9.57	2.1	ng	159951	3	9.92	1519920	20.0