LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092698.D
Acq On : 31 Jan 2017 23:08
Operator : SJ/MA
Sample : I1596-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-16

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	5.127	264	266	269	rBV	840613	893861	15.78%	2.381%
2	5.550	301	303	306	rBV	1790009	2279905	40.25%	6.074%
3	6.579	391	393	396	rBV	1585189	1509684	26.65%	4.022%
4	6.716	402	405	407	rBV	3934234	3734937	65.94%	9.950%
5	6.944	422	425	427	rBV	1191939	1025802	18.11%	2.733%
6	7.104	436	439	441	rBV	3668231	3677535	64.92%	9.797%
7	7.516	472	475	477	rBV	3123116	3433823	60.62%	9.148%
8	7.893	505	508	511	rBV	258733	301229	5.32%	0.803%
9	7.996	513	517	519	rBV	39224	60065	1.06%	0.160%
10	8.236	535	538	540	rVV	1574483	1374642	24.27%	3.662%
11	8.647	572	574	577	rBV	164810	171409	3.03%	0.457%
12	9.322	630	633	635	rBV	4970521	5664387	100.00%	15.090%
13	9.710	665	667	669	rBV	133200	107628	1.90%	0.287%
14	9.996	690	692	695	rVB	1729217	1522172	26.87%	4.055%
15	10.225	710	712	716	rVB	171142	164859	2.91%	0.439%
16	10.419	724	729	731	rBV2	52508	103694	1.83%	0.276%
17	10.499	734	736	742	rVB2	72814	102441	1.81%	0.273%
18	10.785	759	761	764	rBV2	1339584	1847090	32.61%	4.921%
19	10.899	769	771	776	rVB2	78254	101270	1.79%	0.270%
20	11.345	807	810	815	rBV3	76738	122221	2.16%	0.326%
21	11.482	820	822	825	rBV2	1163346	1377809	24.32%	3.671%
22	11.768	845	847	850	rBV	52122	70391	1.24%	0.188%
23	12.888	943	945	948	rVB	89176	77063	1.36%	0.205%
24	13.082	958	962	964	rBV	3891748	5221786	92.19%	13.911%
25	14.122	1050	1053	1056	rBV	1453266	1340758	23.67%	3.572%
26	15.597	1178	1182	1188	rVB	751351	1131087	19.97%	3.013%
27	16.042	1218	1221	1227	rVB	30159	59810	1.06%	0.159%
28	16.557	1263	1266	1271	rVB	29571	58842	1.04%	0.157%

Sum of corrected areas: 37536200

LSC Report - Integrated Chromatogram

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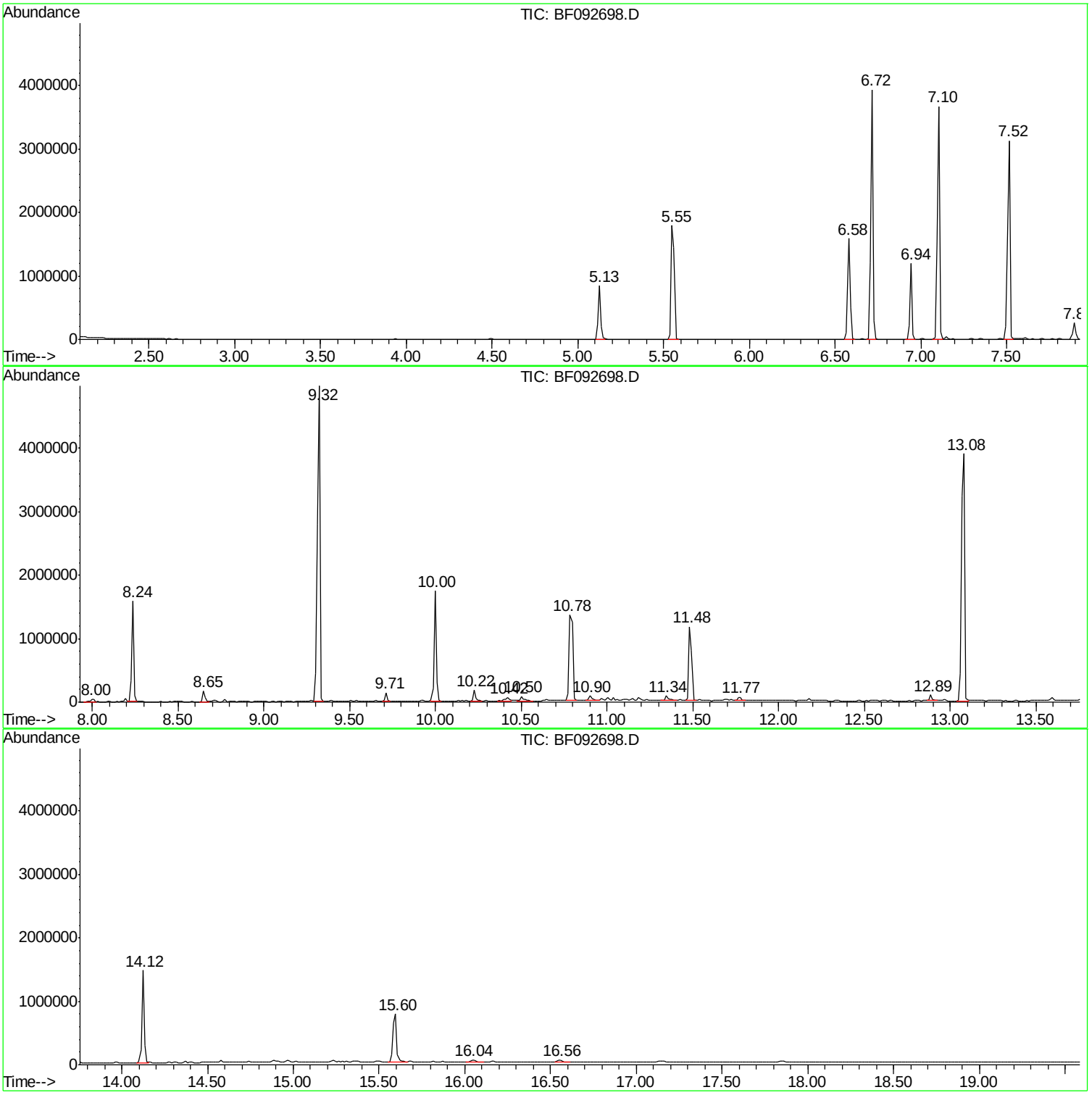
Instrument :
BNA_F
ClientSampleId :
MW-16

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
Data File : BF092698.D
Acq On : 31 Jan 2017 23:08
Operator : SJ/MA
Sample : I1596-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-16

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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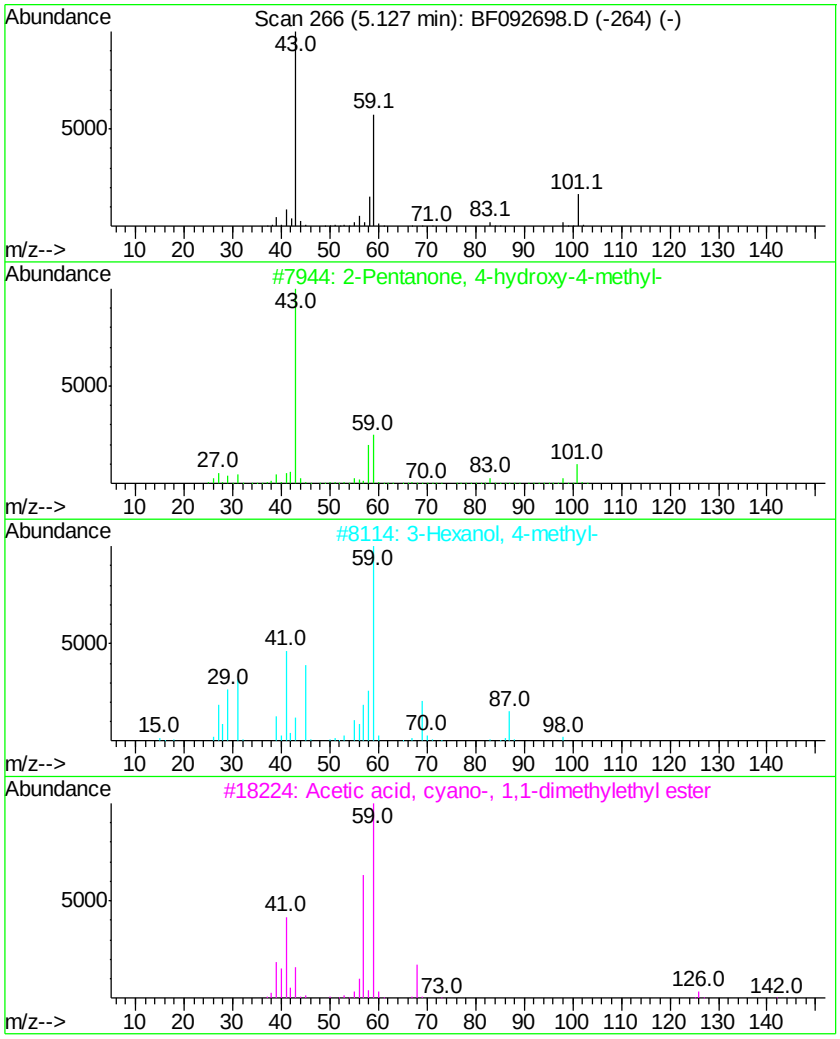
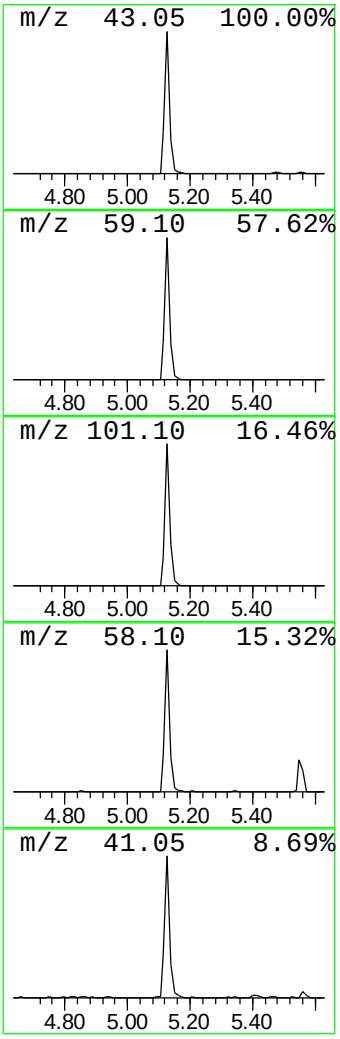
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	17.43 ng	893861	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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Sample : I1596-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-16

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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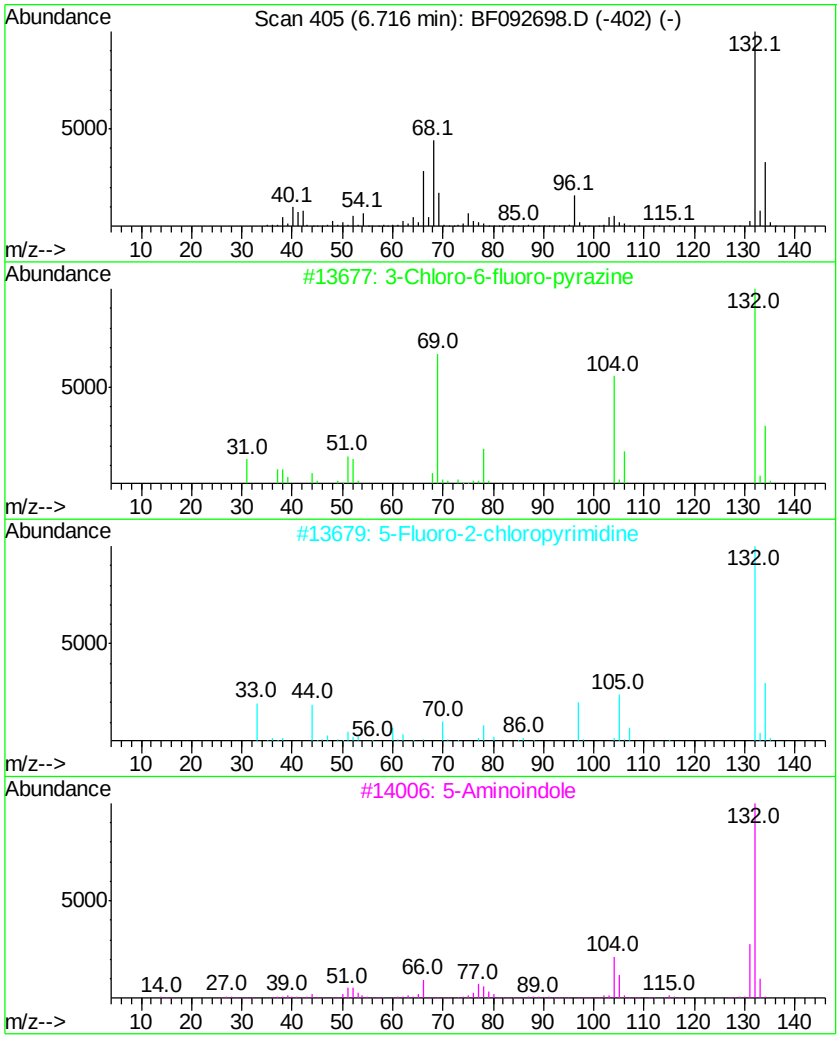
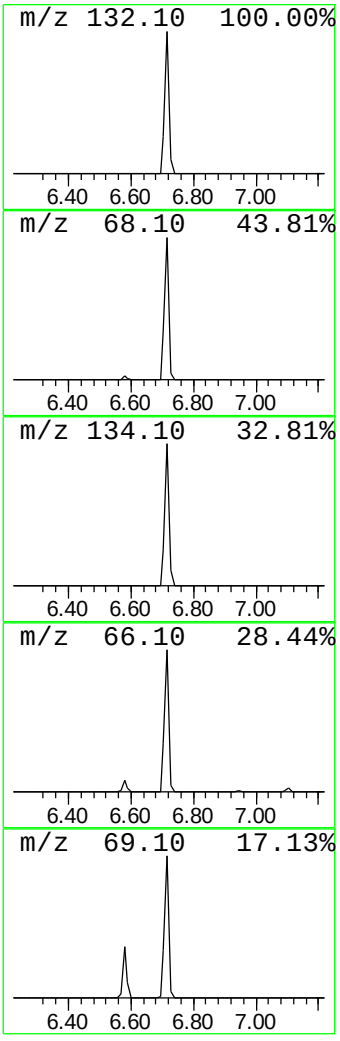
Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	72.82 ng	3734940	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Acq On : 31 Jan 2017 23:08
Operator : SJ/MA
Sample : I1596-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-16

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

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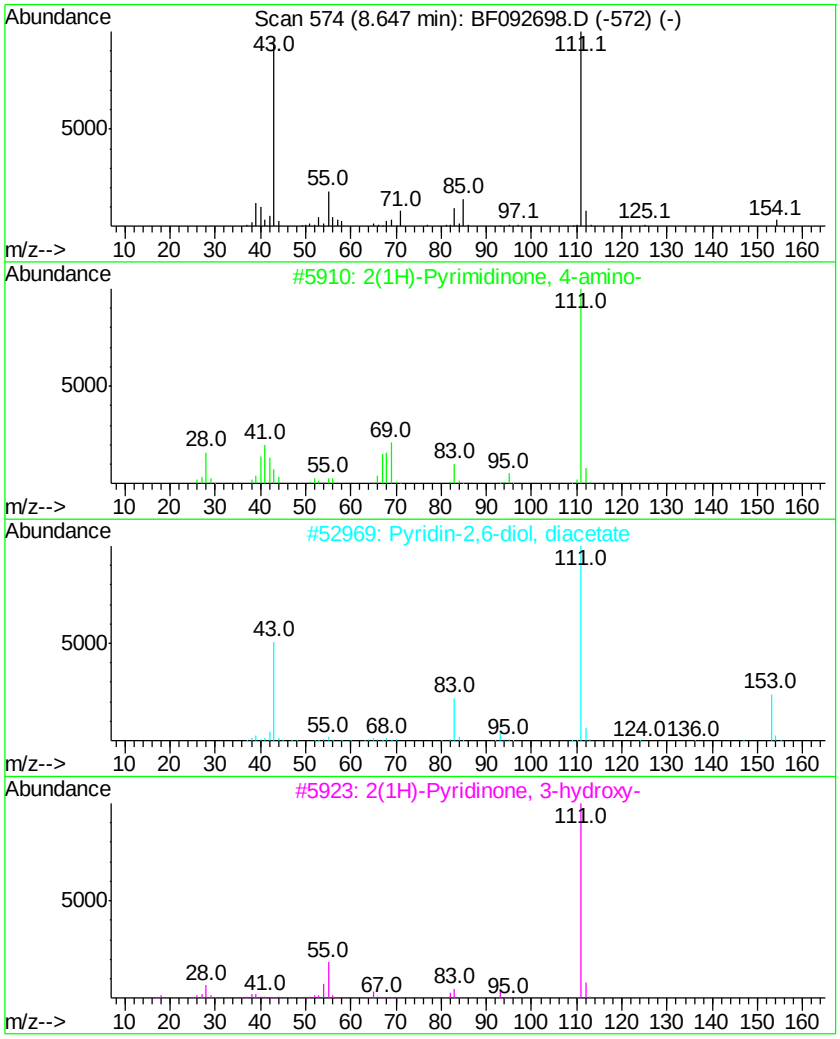
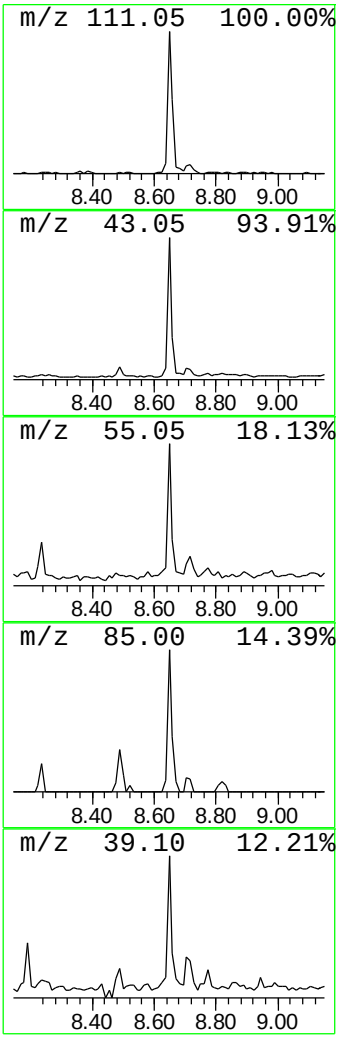
Peak Number 4 unknown8.65 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	2.49 ng	171409	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	47
2	Pyridin-2,6-diol, diacetate	195	C9H9NO4	1000153-09-2	45
3	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	40
4	2-Thiophenecarboxylic acid, 4-me...	212	C11H16O2S	1000278-88-0	38
5	3-Aminopyrazine 1-oxide	111	C4H5N3O	006863-77-0	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF013117\
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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-16

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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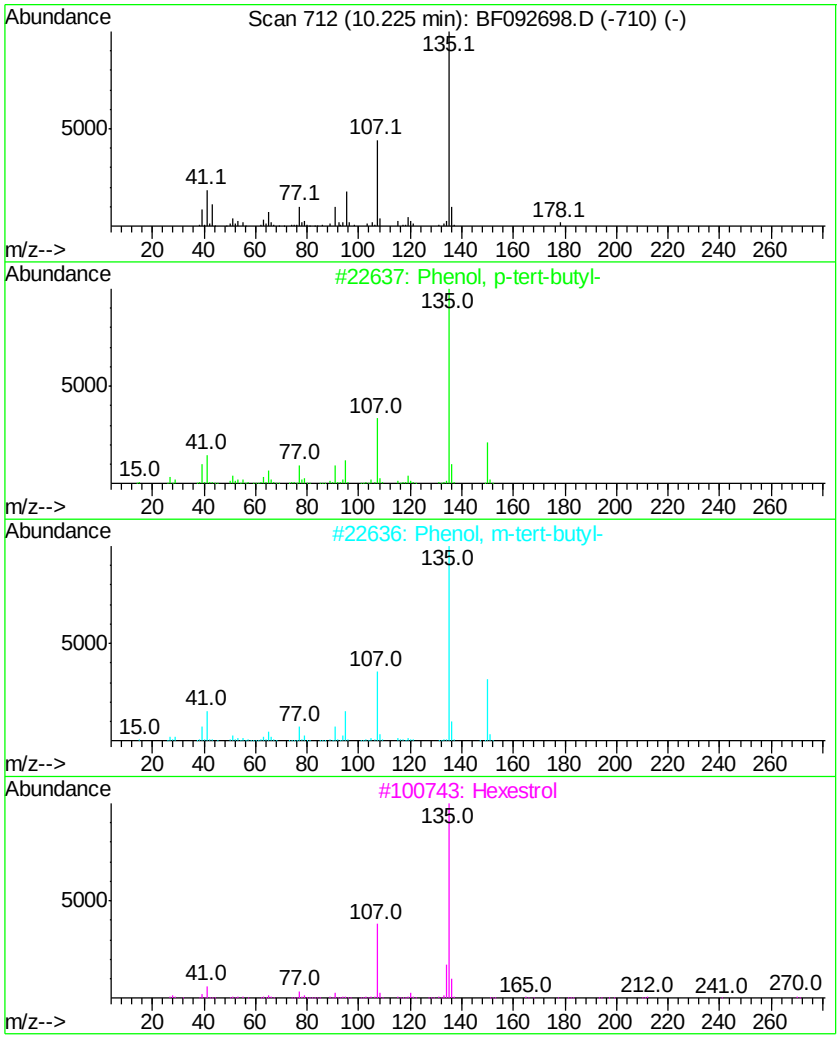
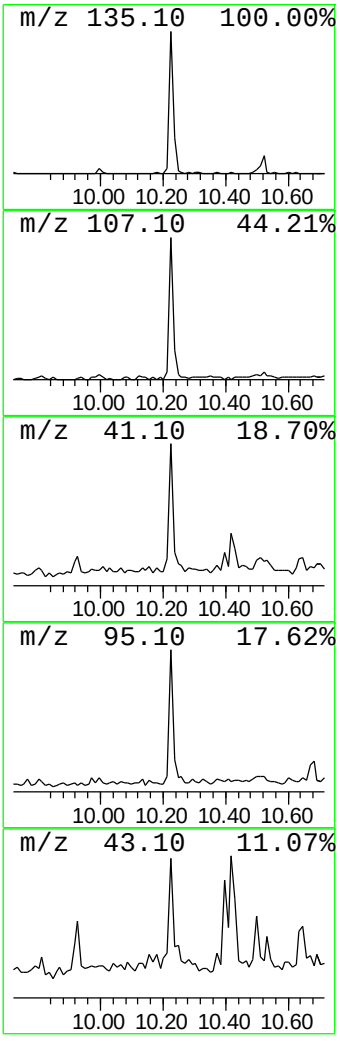
Peak Number 5 Phenol, p-tert-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.22	2.17 ng	164859	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	83
3	Hexestrol	270	C18H22O2	005635-50-7	72
4	Phenol, 4,4'-(1,2-diethyl-1,2-et...	270	C18H22O2	000084-16-2	64
5	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF013117\
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Operator : SJ/MA
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ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-16

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.13	17.4	ng	893861	1	6.94	1025800	20.0
unknown6.72	6.72	72.8	ng	3734940	1	6.94	1025800	20.0
unknown8.65	8.65	2.5	ng	171409	2	8.24	1374640	20.0
Phenol, p-tert-bu...	10.22	2.2	ng	164859	3	10.00	1522170	20.0