LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032116\
Data File : BF085651.D
Acq On : 22 Mar 2016 7:07
Operator : UM/SJ
Sample : H1838-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

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-BF031816.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	2.412	6	11	18	rVB3	13668	53235	1.73%	0.190%
2	2.675	32	34	41	rVB	46740	70992	2.30%	0.253%
3	5.041	238	241	249	rBV	518667	827464	26.82%	2.948%
4	5.418	272	274	275	rBV	51255	88807	2.88%	0.316%
5	5.453	275	277	279	rVB	2506777	2558226	82.92%	9.113%
6	5.681	294	297	299	rBV	101267	103048	3.34%	0.367%
7	5.853	310	312	315	rBV	62242	56148	1.82%	0.200%
8	6.367	354	357	358	rBV	88845	78745	2.55%	0.280%
9	6.401	358	360	362	rVV	23772	31678	1.03%	0.113%
10	6.481	364	367	369	rVV	2341611	2755160	89.30%	9.814%
11	6.527	369	371	373	rVV	97254	96713	3.13%	0.345%
12	6.607	376	378	381	rVV	2373940	2819163	91.37%	10.042%
13	6.664	381	383	386	rVB	159546	140374	4.55%	0.500%
14	6.836	396	398	400	rBV	559755	742235	24.06%	2.644%
15	6.904	400	404	408	rVB	68892	121370	3.93%	0.432%
16	6.996	410	412	415	rBV	2318414	2341350	75.89%	8.340%
17	7.167	425	427	431	rVB	37564	43940	1.42%	0.157%
18	7.407	445	448	450	rVB	1915279	1882021	61.00%	6.704%
19	7.636	467	468	474	rVB2	28530	40674	1.32%	0.145%
20	7.796	479	482	485	rVB2	45517	53003	1.72%	0.189%
21	7.864	485	488	490	rBV	165666	160129	5.19%	0.570%
22	7.967	493	497	499	rVV	135354	124863	4.05%	0.445%
23	8.127	508	511	514	rBV	1131987	1340554	43.45%	4.775%
24	8.322	526	528	530	rVB	47509	40664	1.32%	0.145%
25	8.367	530	532	534	rBV	34603	38982	1.26%	0.139%
26	8.516	543	545	547	rBV	31460	31569	1.02%	0.112%
27	8.630	553	555	557	rVV	166173	138275	4.48%	0.493%
28	8.790	567	569	571	rVB	85757	88113	2.86%	0.314%
29	8.836	571	573	575	rVB	163619	147594	4.78%	0.526%
30	8.939	579	582	584	rBV2	145982	178650	5.79%	0.636%
31	9.065	591	593	598	rBV3	20546	37269	1.21%	0.133%
32	9.202	603	605	608	rVV	3162701	3085269	100.00%	10.990%
33	9.305	610	614	616	rVB3	36222	60884	1.97%	0.217%
34	9.350	616	618	619	rBV	51110	42752	1.39%	0.152%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H1838-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

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-BF031816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.373	619	620	625	rVB2	18985	39209	1.27%	0.140%
36	9.465	625	628	631	rBV2	49484	74899	2.43%	0.267%
37	9.533	631	634	636	rBV	79946	133191	4.32%	0.474%
38	9.659	643	645	647	rVB	40213	53503	1.73%	0.191%
39	9.876	662	664	666	rBV	1047803	990123	32.09%	3.527%
40	9.910	666	667	670	rVB	41159	35865	1.16%	0.128%
41	10.665	730	733	736	rBV	1590727	1643420	53.27%	5.854%
42	11.362	792	794	796	rBV	925443	824481	26.72%	2.937%
43	12.768	915	917	919	rBV	36525	31393	1.02%	0.112%
44	12.951	930	933	935	rBV	2108130	2520079	81.68%	8.977%
45	13.991	1022	1024	1027	rBV	679082	647157	20.98%	2.305%
46	15.419	1146	1149	1157	rBV	538447	660147	21.40%	2.352%

Sum of corrected areas: 28073380

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Instrument :
BNA_F
ClientSampleId :
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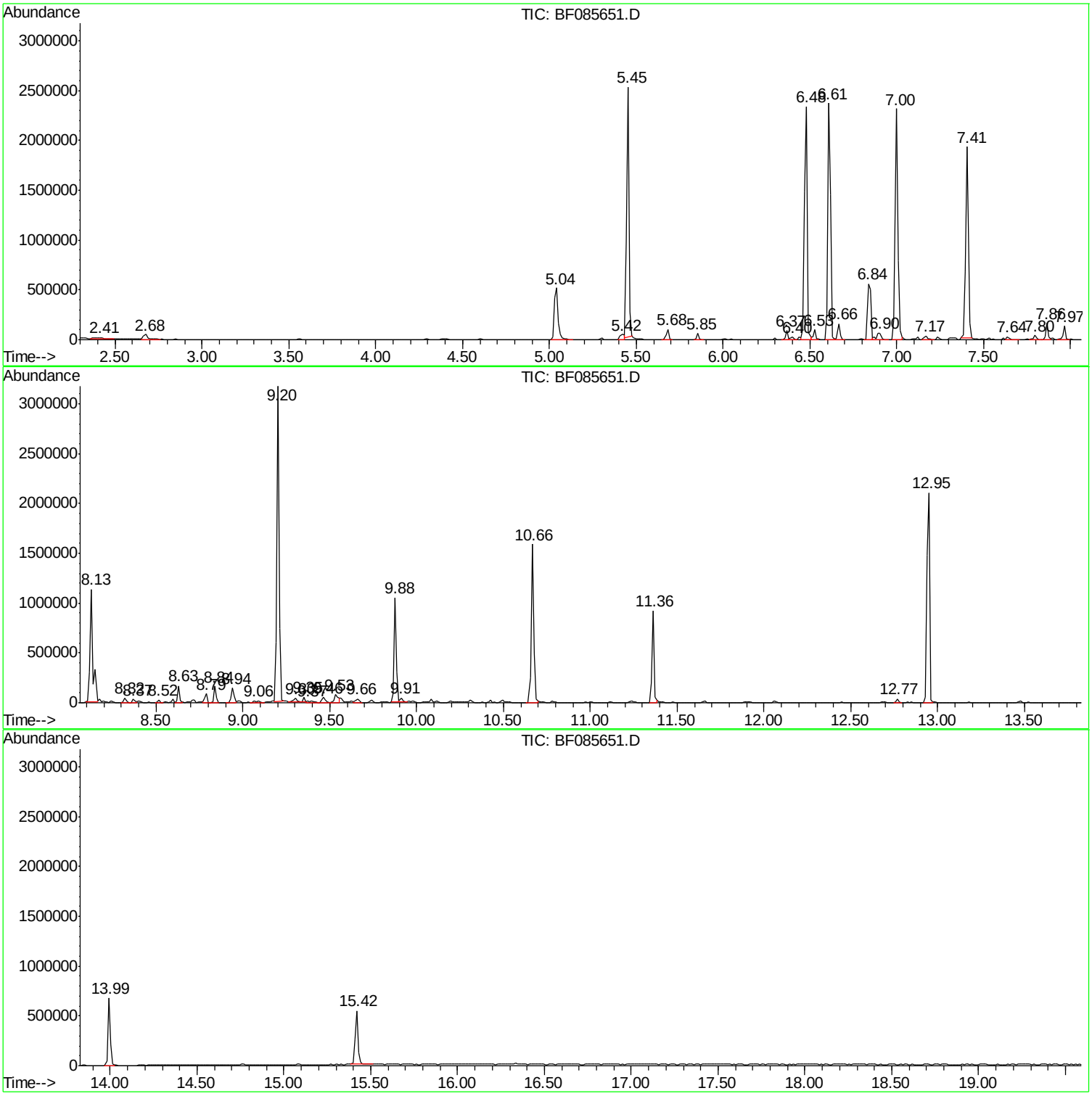
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Operator : UM/SJ
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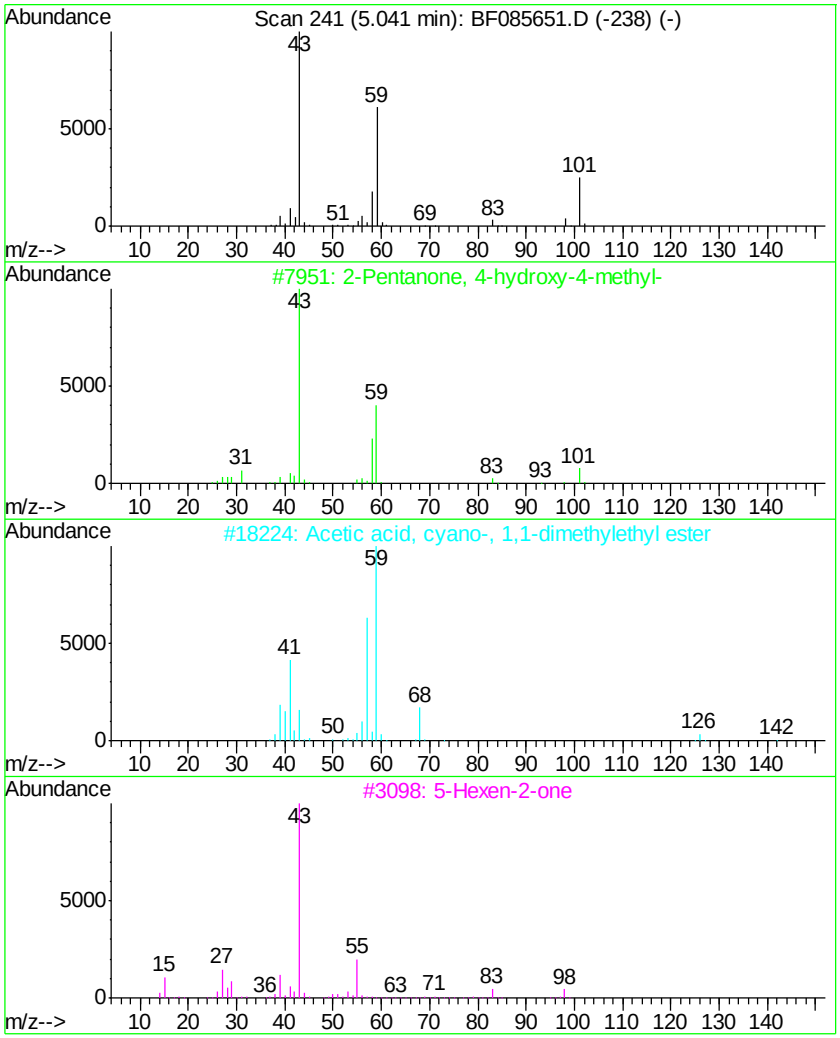
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

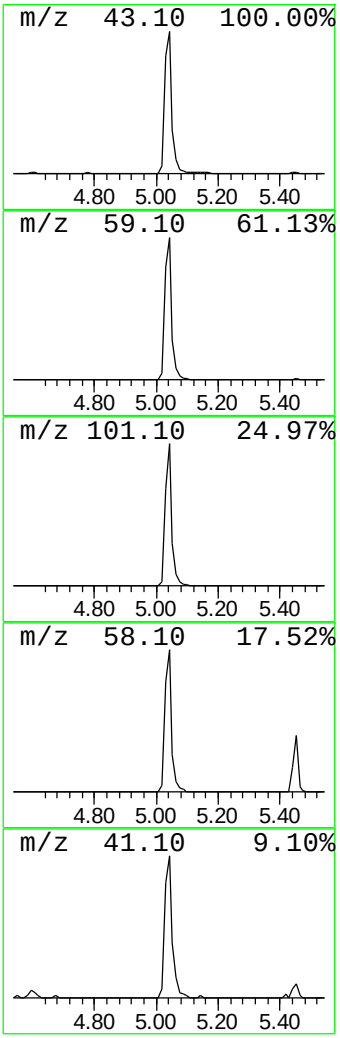
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	22.30 ng	827464	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

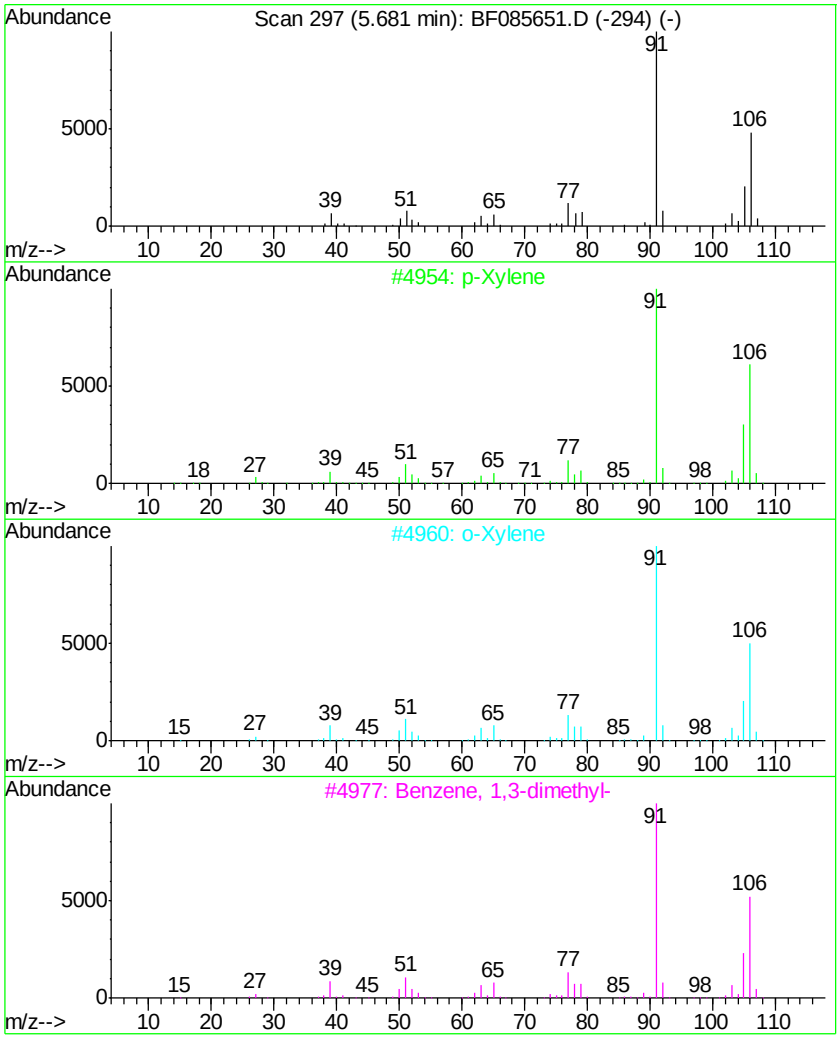
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

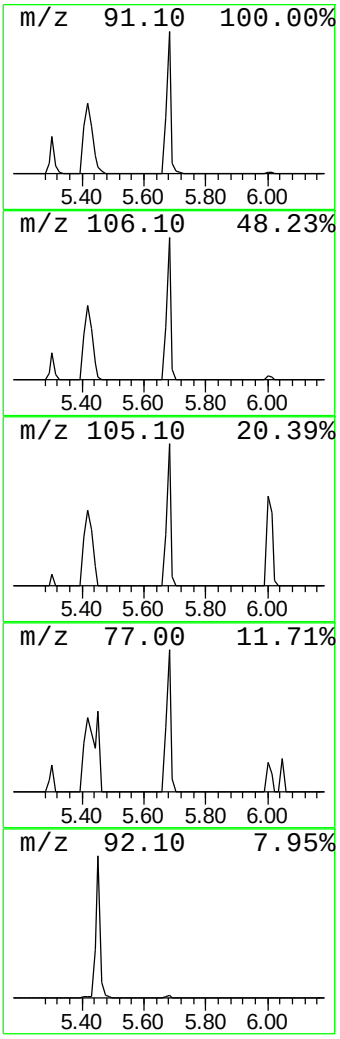
****

Peak Number 2 p-Xylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	2.78 ng	103048	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Xylene	106	C8H10	000106-42-3	97
2	o-Xylene	106	C8H10	000095-47-6	97
3	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	87
5	Ethylbenzene	106	C8H10	000100-41-4	80





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Sample : H1838-03
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ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

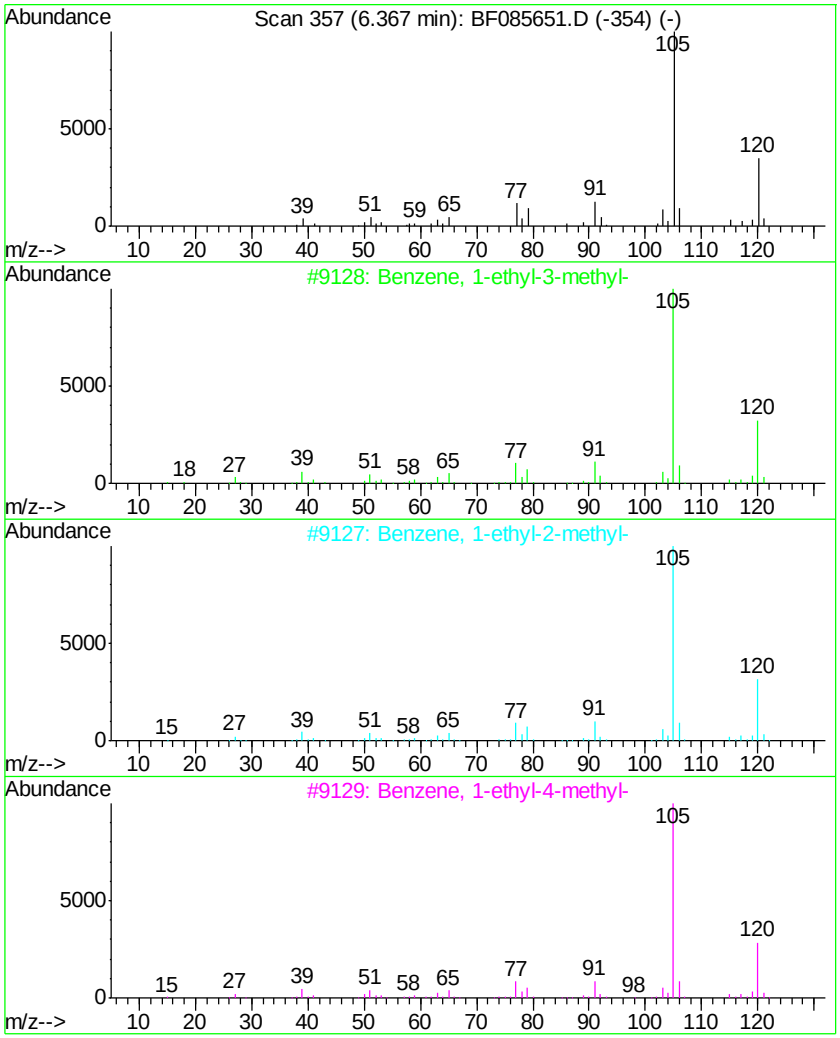
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

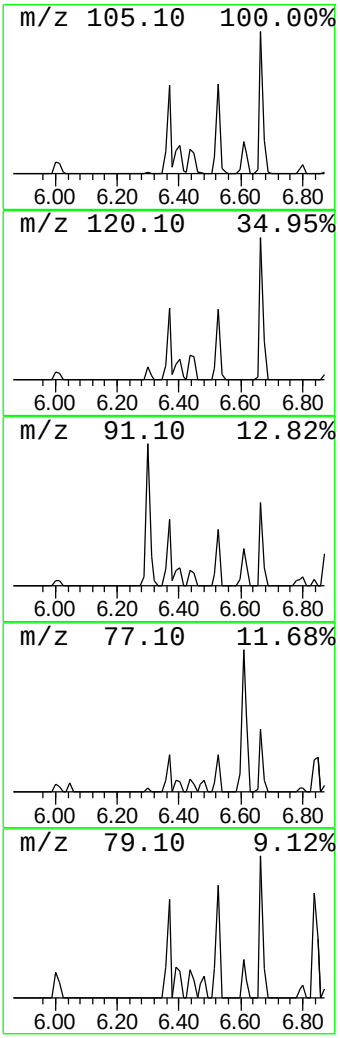
****

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	2.12 ng	78745	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





Library Search Compound Report

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ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

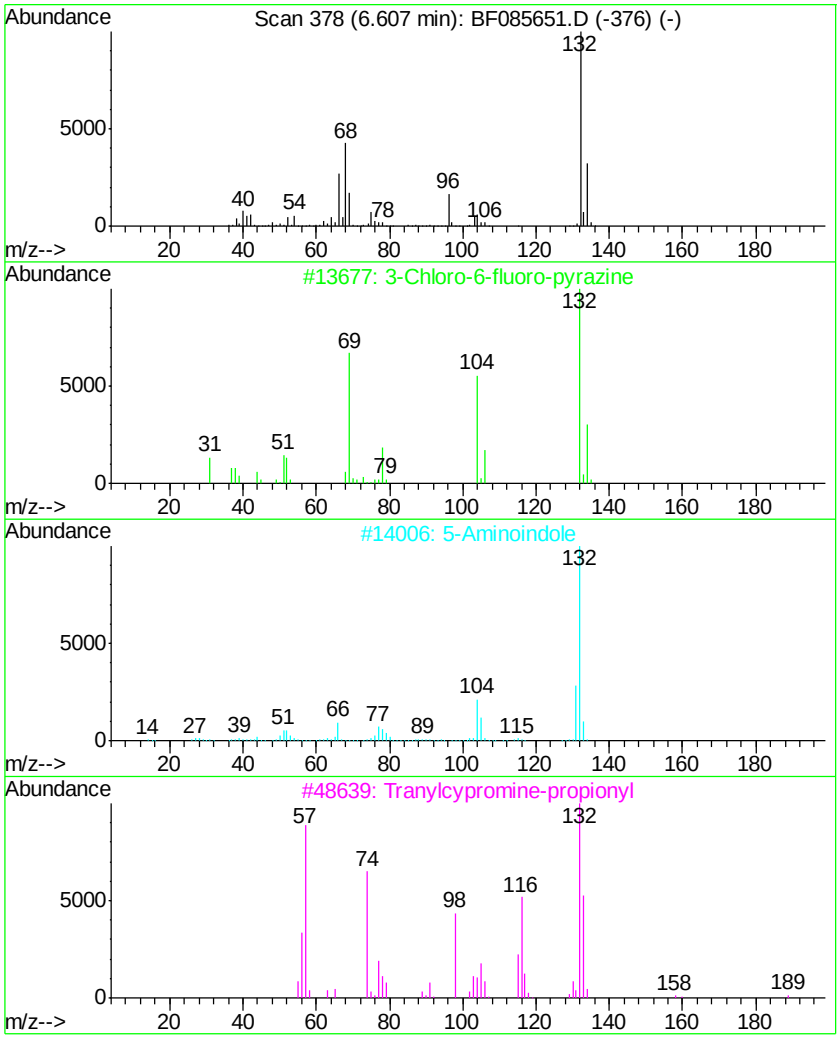
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

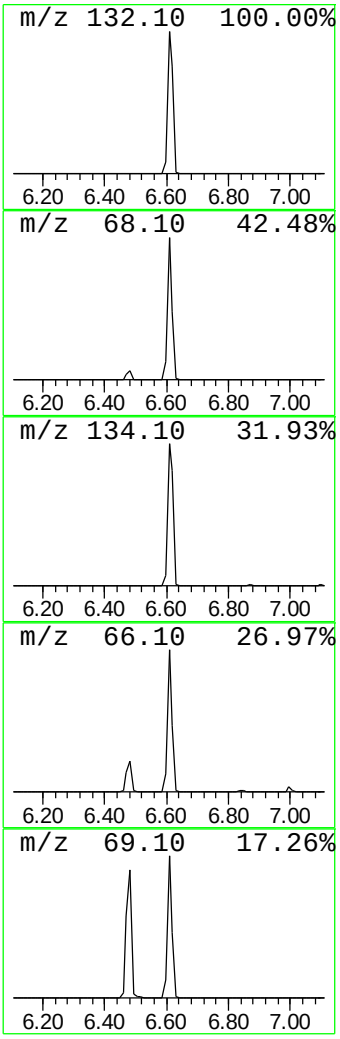
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	75.96 ng	2819160	1,4-Dichlorobenzene-d4	6.85

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
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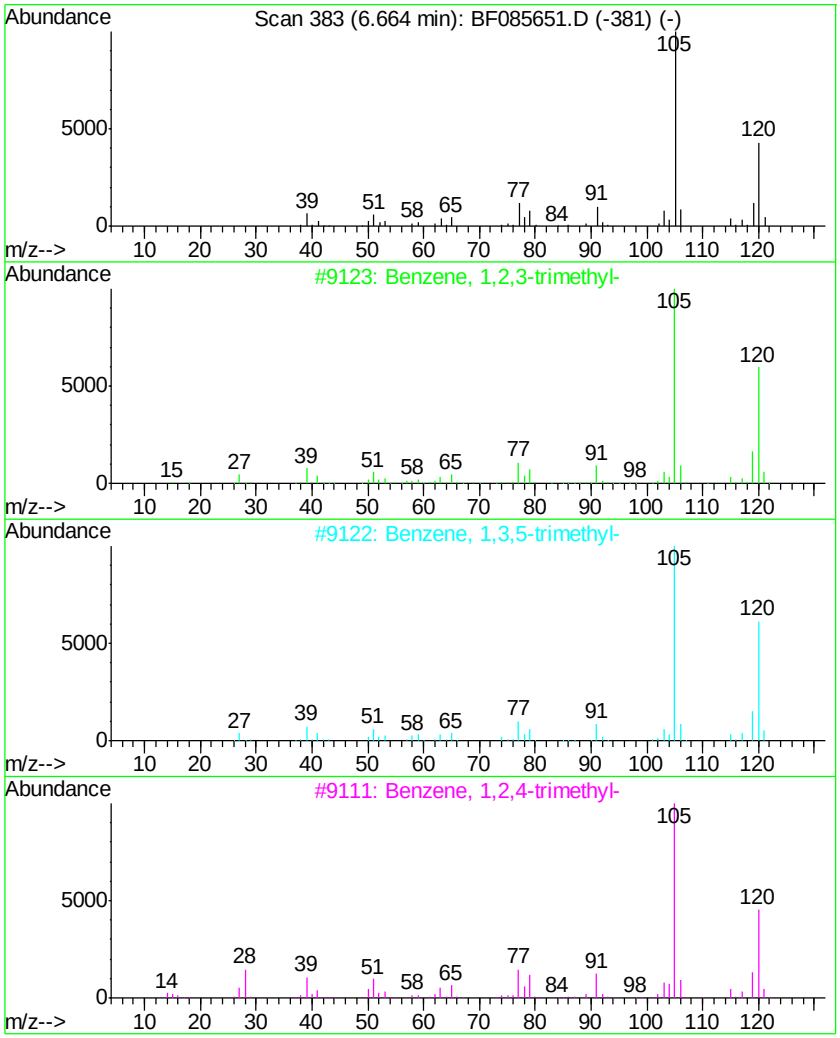
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

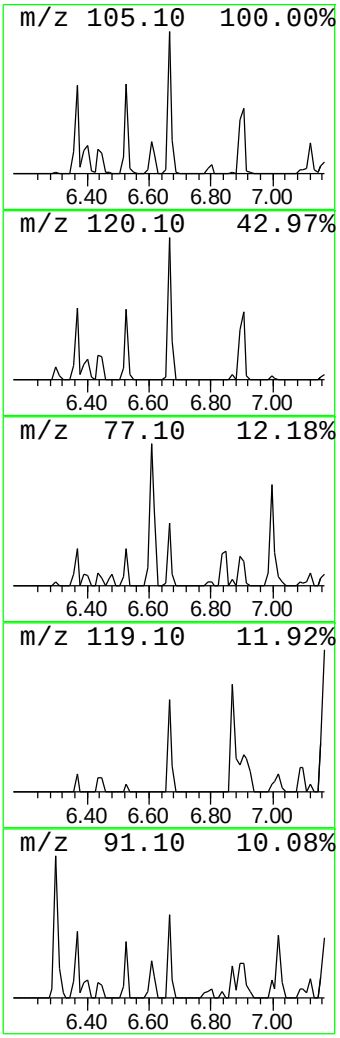
****

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	3.78 ng	140374	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	97
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Library Search Compound Report

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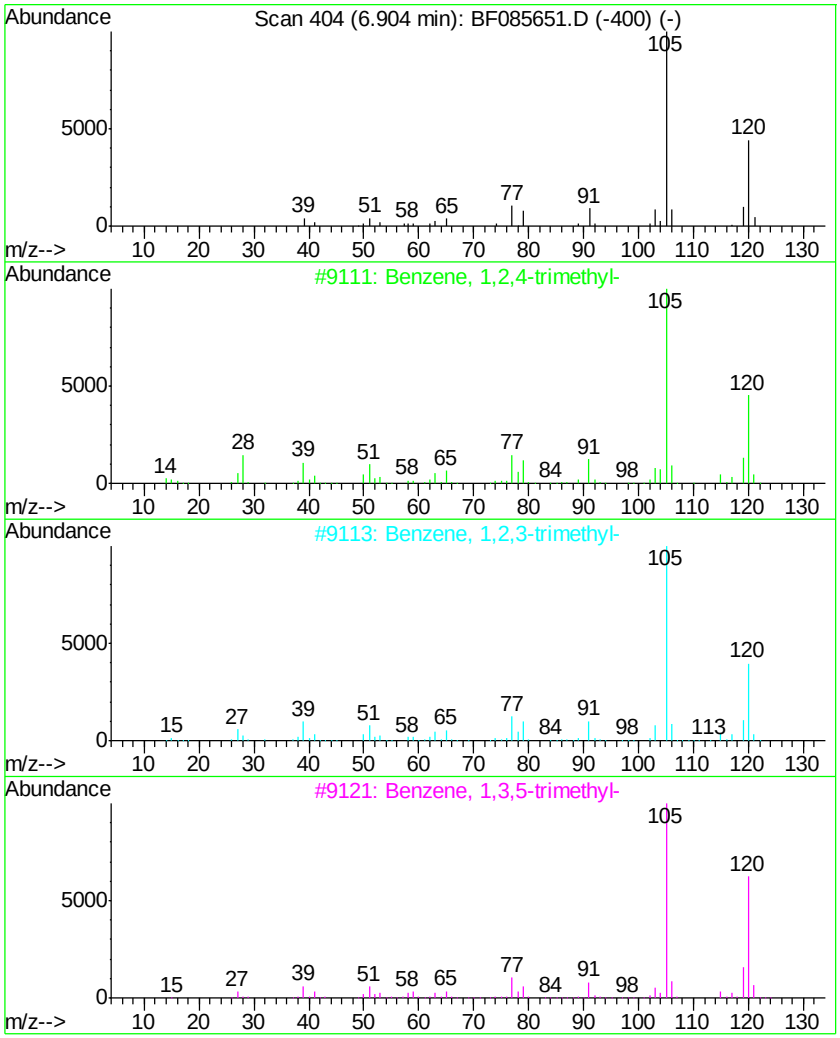
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

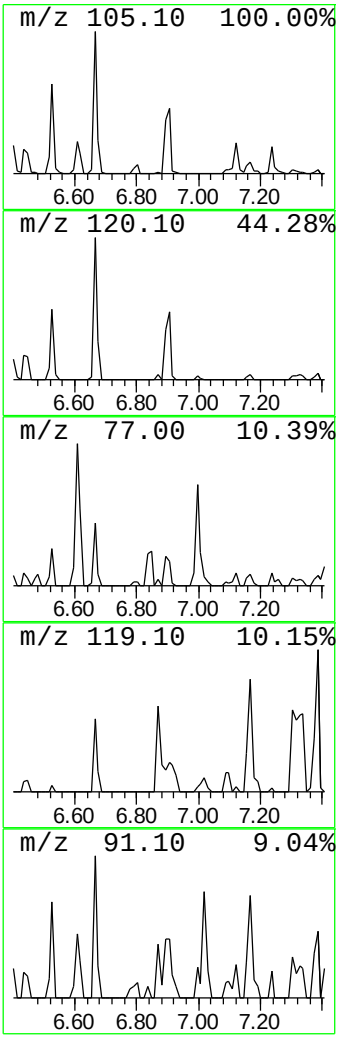
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	3.27 ng	121370	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	86





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

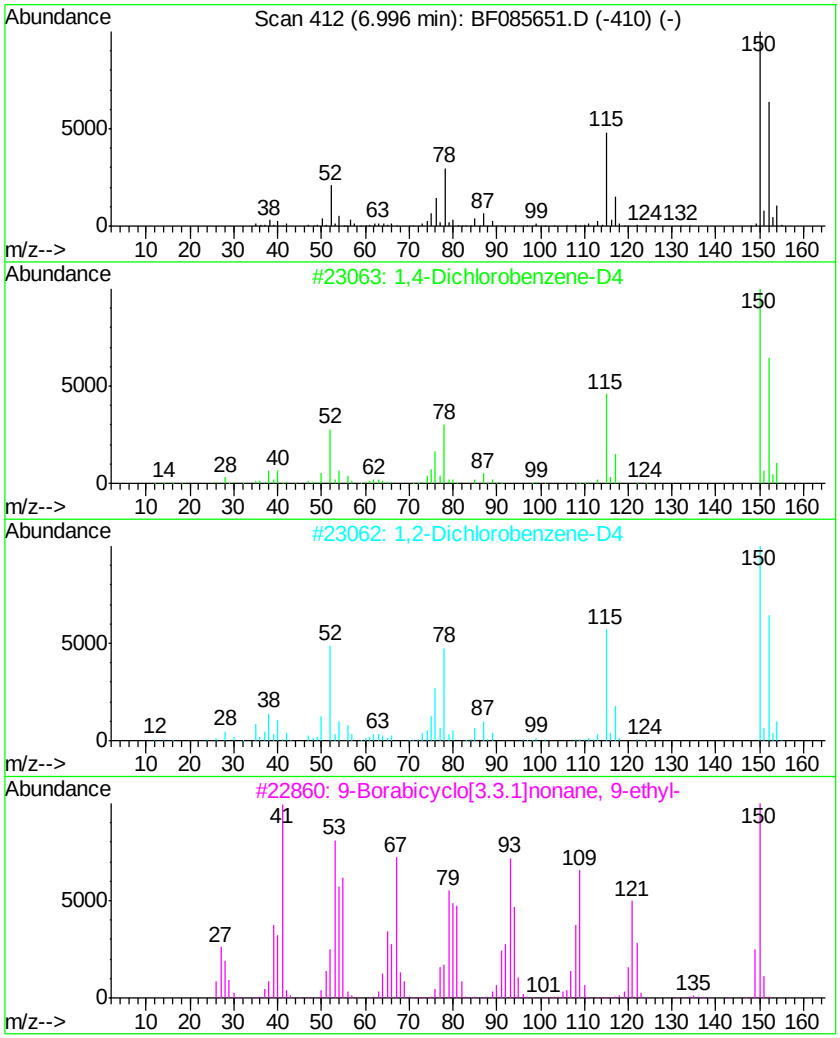
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

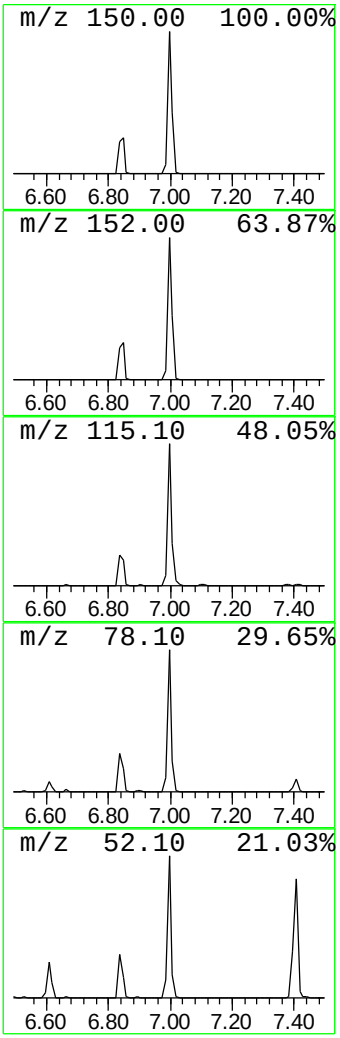
****

Peak Number 7 1,4-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.00	63.09 ng	2341350	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	95
2	1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94
3	9-Borabicyclo[3.3.1]nonane, 9-et...	150	C10H19B	052102-17-7	38
4	2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	35
5	2,3,5-Tri-O-p-nitrobenzoyl-.alph...	606	C27H18N4O13	1000129-91-5	10





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Data File : BF085651.D
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Operator : UM/SJ
Sample : H1838-03
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Instrument :
BNA_F
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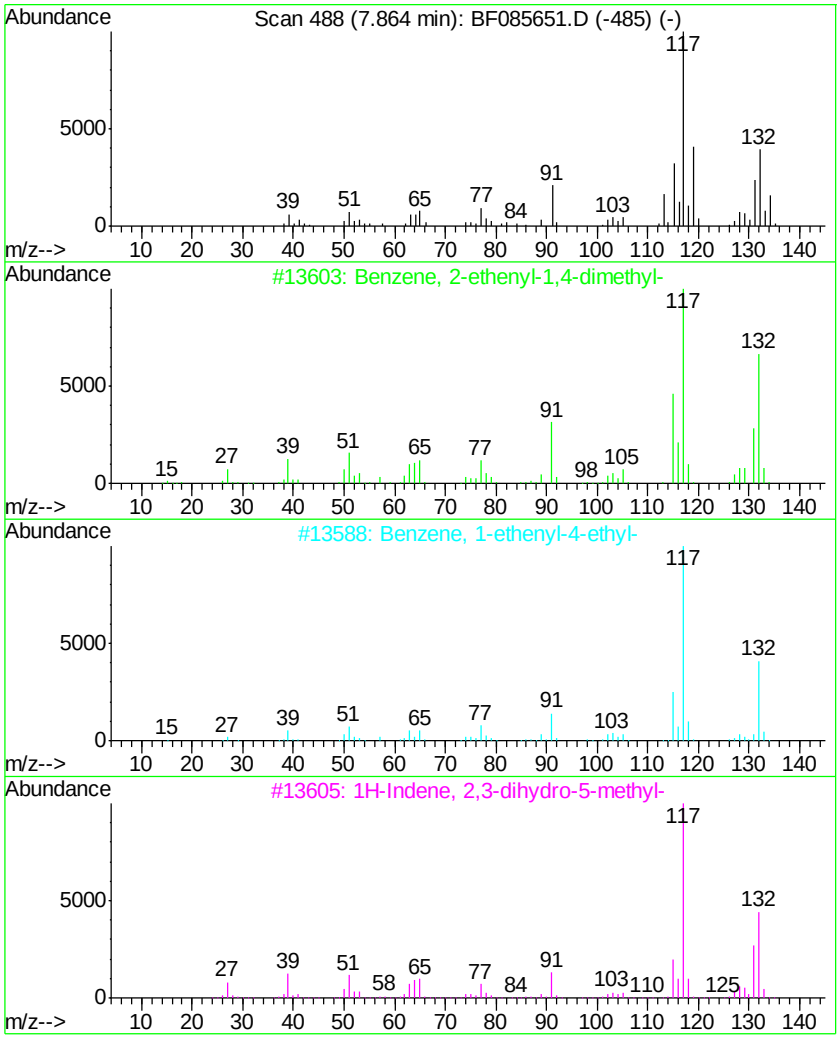
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

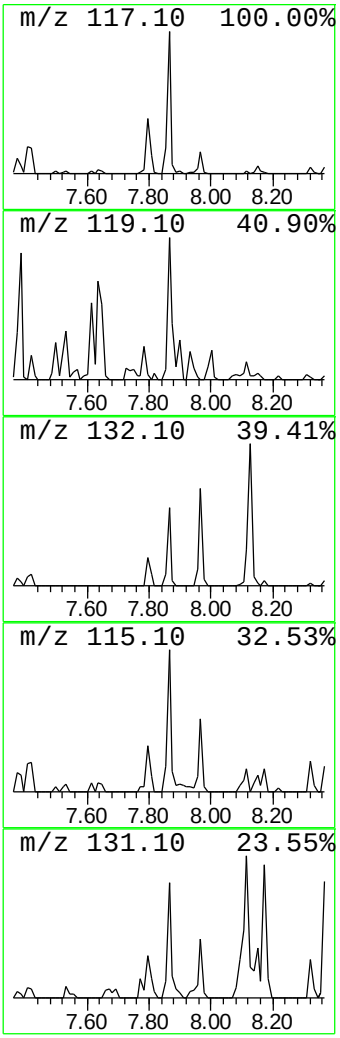
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.86	2.39 ng	160129	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	91
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	76
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	70
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70





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Data File : BF085651.D
Acq On : 22 Mar 2016 7:07
Operator : UM/SJ
Sample : H1838-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

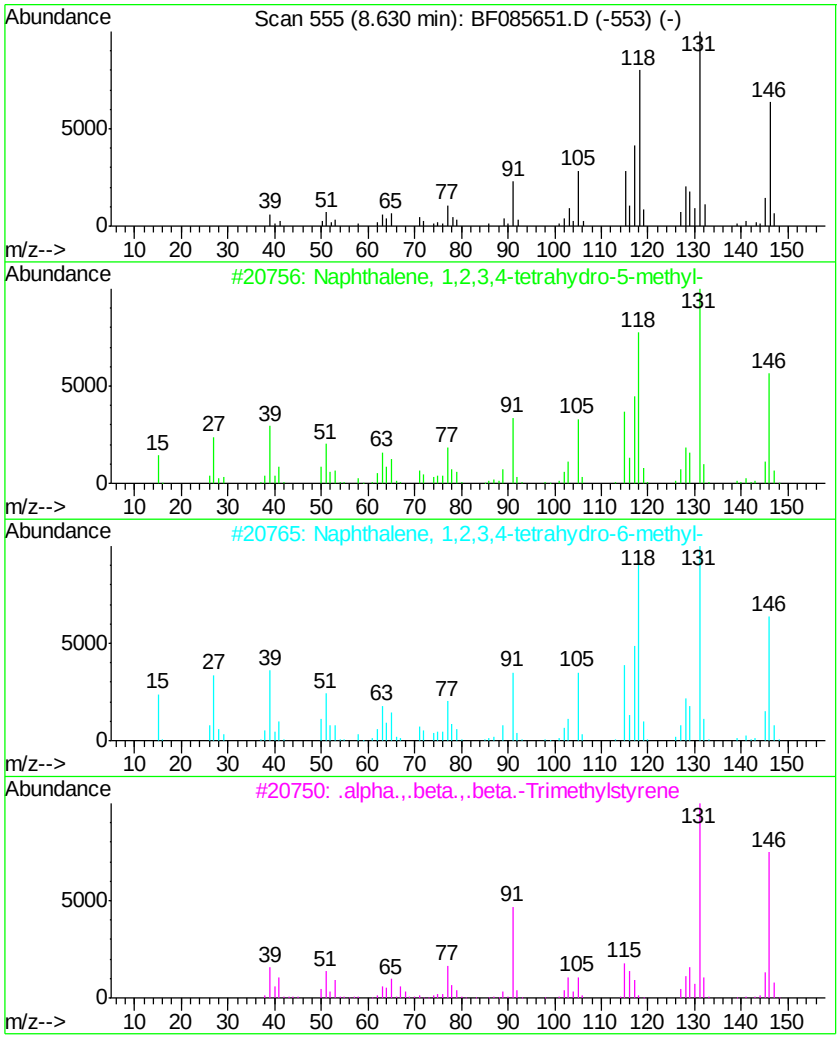
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

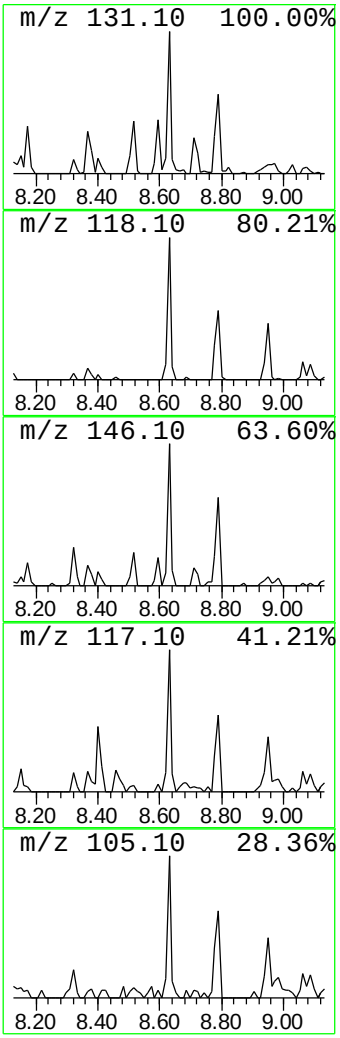
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	2.06 ng	138275	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	96
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	96
3	.alpha.,.beta.,.beta.-Trimethyls...	146	C11H14	000769-57-3	87
4	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	60
5	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	60





Library Search Compound Report

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Data File : BF085651.D
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Sample : H1838-03
Misc :
ALS Vial : 34 Sample Multiplier: 1

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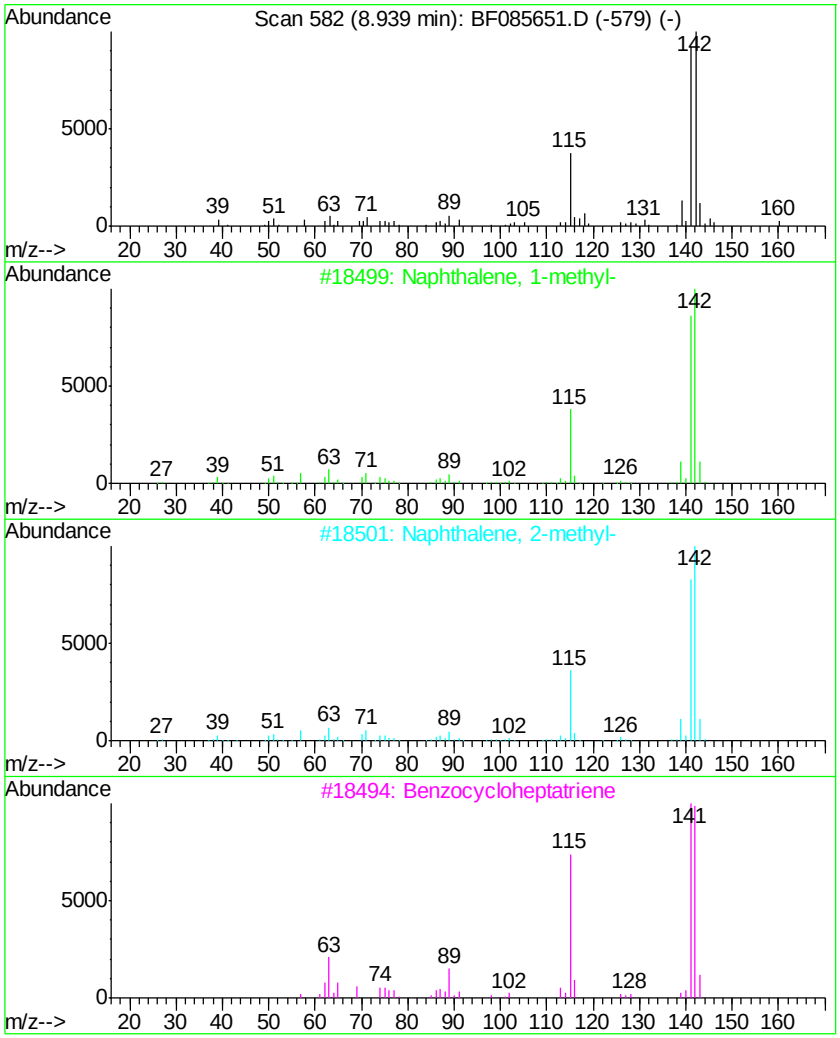
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

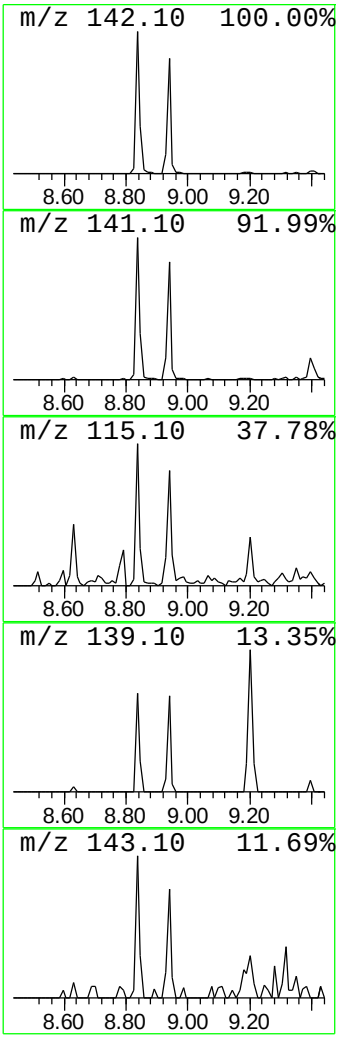
****

Peak Number 10 Naphthalene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.94	2.67 ng	178650	Naphthalene-d8	8.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	90
4	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	90
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90





Library Search Compound Report

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Sample : H1838-03
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ALS Vial : 34 Sample Multiplier: 1

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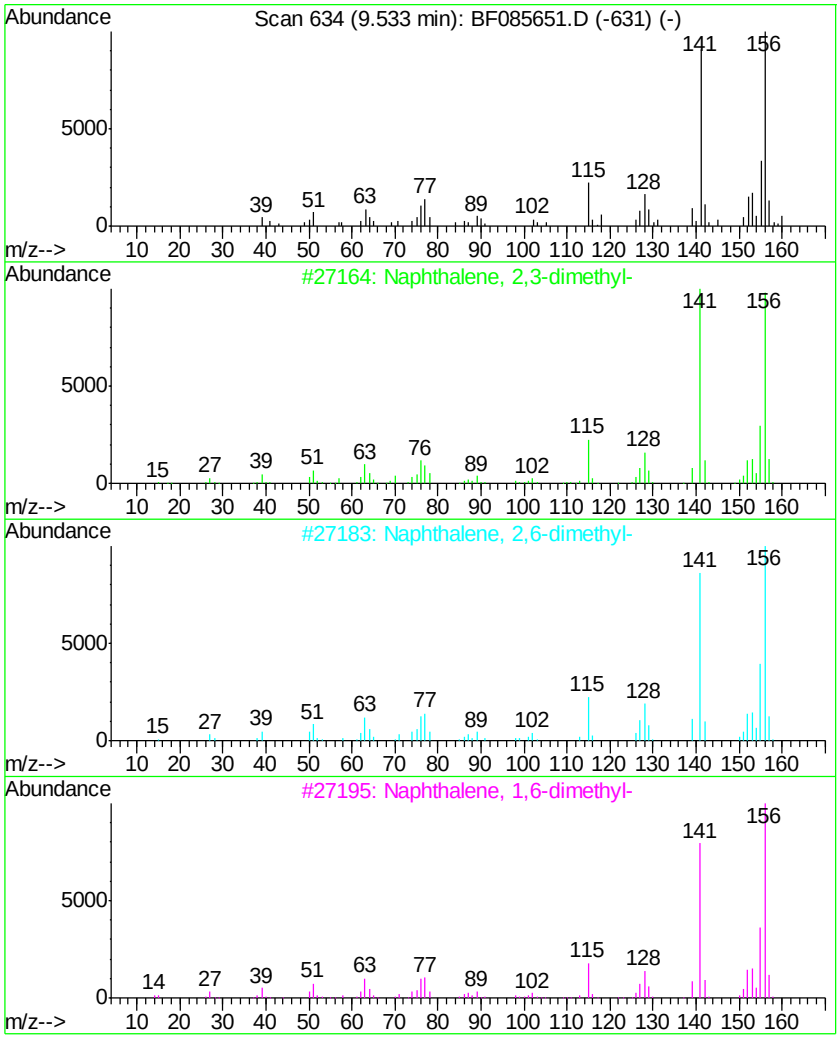
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

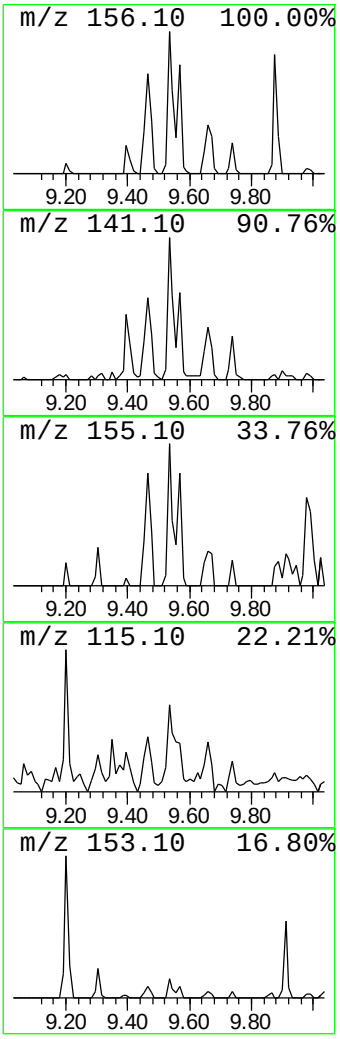
****

Peak Number 11 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.53	2.69 ng	133191	Acenaphthene-d10	9.88

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	98
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
5	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	22.3	ng	827464	1	6.85	742235	20.0
p-Xylene	5.68	2.8	ng	103048	1	6.85	742235	20.0
Benzene, 1-ethyl-...	6.37	2.1	ng	78745	1	6.85	742235	20.0
3-Chloro-6-fluoro...	6.61	76.0	ng	2819160	1	6.85	742235	20.0
Benzene, 1,2,3-tr...	6.66	3.8	ng	140374	1	6.85	742235	20.0
Benzene, 1,2,4-tr...	6.90	3.3	ng	121370	1	6.85	742235	20.0
1,4-Dichlorobenze...	7.00	63.1	ng	2341350	1	6.85	742235	20.0
Benzene, 2-etheny...	7.86	2.4	ng	160129	2	8.13	1340550	20.0
Naphthalene, 1,2,...	8.63	2.1	ng	138275	2	8.13	1340550	20.0
Naphthalene, 1-me...	8.94	2.7	ng	178650	2	8.13	1340550	20.0
Naphthalene, 2,3-...	9.53	2.7	ng	133191	3	9.88	990123	20.0