LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

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-BF060716.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	1.735	11	13	22	rVV	459030	985131	30.48%	3.331%
2	1.861	22	24	63	rVB	1488585	3232474	100.00%	10.930%
3	4.970	294	296	299	rBV	418879	506717	15.68%	1.713%
4	5.061	301	304	306	rVB	173516	171070	5.29%	0.578%
5	5.359	328	330	331	rBV	54020	56301	1.74%	0.190%
6	5.393	331	333	336	rVB	1122887	1290392	39.92%	4.363%
7	6.433	422	424	426	rVV	1036572	961065	29.73%	3.250%
8	6.479	426	428	430	rVV	36630	32515	1.01%	0.110%
9	6.570	433	436	438	rVV	2169535	2397672	74.17%	8.107%
10	6.627	438	441	443	rVB	128261	144231	4.46%	0.488%
11	6.799	454	456	458	rBV	748801	613230	18.97%	2.073%
12	6.856	460	461	463	rBV	68335	59929	1.85%	0.203%
13	6.959	467	470	472	rBV	2174287	2168078	67.07%	7.331%
14	7.130	483	485	489	rBV2	23560	45209	1.40%	0.153%
15	7.370	502	506	508	rBV	1670066	2054320	63.55%	6.946%
16	7.450	510	513	515	rVB2	48182	50498	1.56%	0.171%
17	7.576	521	524	525	rBV	36246	35475	1.10%	0.120%
18	7.599	525	526	529	rBV3	44419	74891	2.32%	0.253%
19	7.759	537	540	543	rBV3	21179	44566	1.38%	0.151%
20	7.827	543	546	548	rBV	96840	99586	3.08%	0.337%
21	8.090	566	569	572	rVB	801902	1049294	32.46%	3.548%
22	8.216	578	580	582	rBV2	26132	45893	1.42%	0.155%
23	8.376	590	594	595	rBV3	32124	67581	2.09%	0.229%
24	8.445	597	600	602	rVV2	89749	175463	5.43%	0.593%
25	8.548	604	609	611	rVV3	81557	166958	5.17%	0.565%
26	8.593	611	613	616	rVV3	35685	77980	2.41%	0.264%
27	8.662	618	619	622	rVB3	51772	52875	1.64%	0.179%
28	8.799	629	631	633	rVB	63701	57629	1.78%	0.195%
29	8.902	637	640	642	rBV	89062	95866	2.97%	0.324%
30	9.165	660	663	666	rBV	2520828	3202996	99.09%	10.830%
31	9.359	679	680	683	rVB	31281	37642	1.16%	0.127%
32	9.428	683	686	688	rBV	59538	81977	2.54%	0.277%
33	9.496	690	692	694	rVV	107486	143235	4.43%	0.484%
34	9.531	694	695	697	rVV2	52542	42522	1.32%	0.144%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.622	701	703	705	rVB	27394	48382	1.50%	0.164%
36	9.839	719	722	724	rBV	1002538	958955	29.67%	3.242%
37	9.873	724	725	729	rVB2	40578	46767	1.45%	0.158%
38	9.942	729	731	734	rBV	21741	33902	1.05%	0.115%
39	10.045	737	740	741	rBV	45635	46888	1.45%	0.159%
40	10.079	741	743	747	rVB2	36627	49262	1.52%	0.167%
41	10.159	747	750	751	rBV2	30998	33315	1.03%	0.113%
42	10.228	754	756	757	rBV	229307	208938	6.46%	0.706%
43	10.262	757	759	763	rVB	92370	98986	3.06%	0.335%
44	10.365	766	768	771	rVB2	44259	60947	1.89%	0.206%
45	10.456	773	776	777	rBV2	32683	50896	1.57%	0.172%
46	10.628	788	791	794	rBV	1646651	1904560	58.92%	6.440%
47	11.325	849	852	854	rBV	960099	1026881	31.77%	3.472%
48	12.788	978	980	983	rBV	87699	107017	3.31%	0.362%
49	12.914	988	991	993	rBV	2824828	3051365	94.40%	10.317%
50	13.817	1067	1070	1078	rBV3	23022	54222	1.68%	0.183%
51	13.954	1080	1082	1084	rBV	914506	877555	27.15%	2.967%
52	15.371	1203	1206	1209	rBV	394374	594790	18.40%	2.011%

Sum of corrected areas: 29574889

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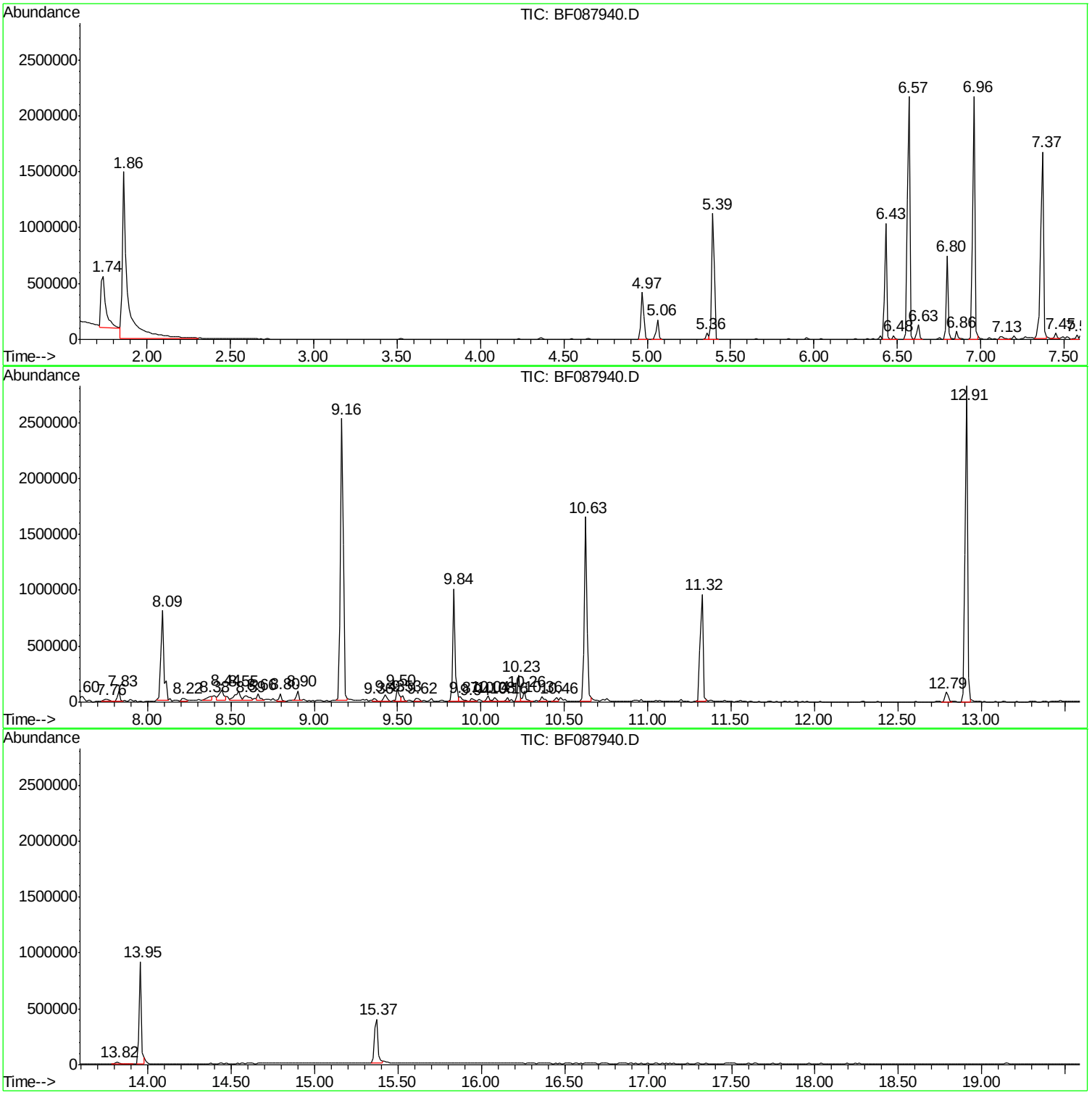
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP16-JMW0882

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

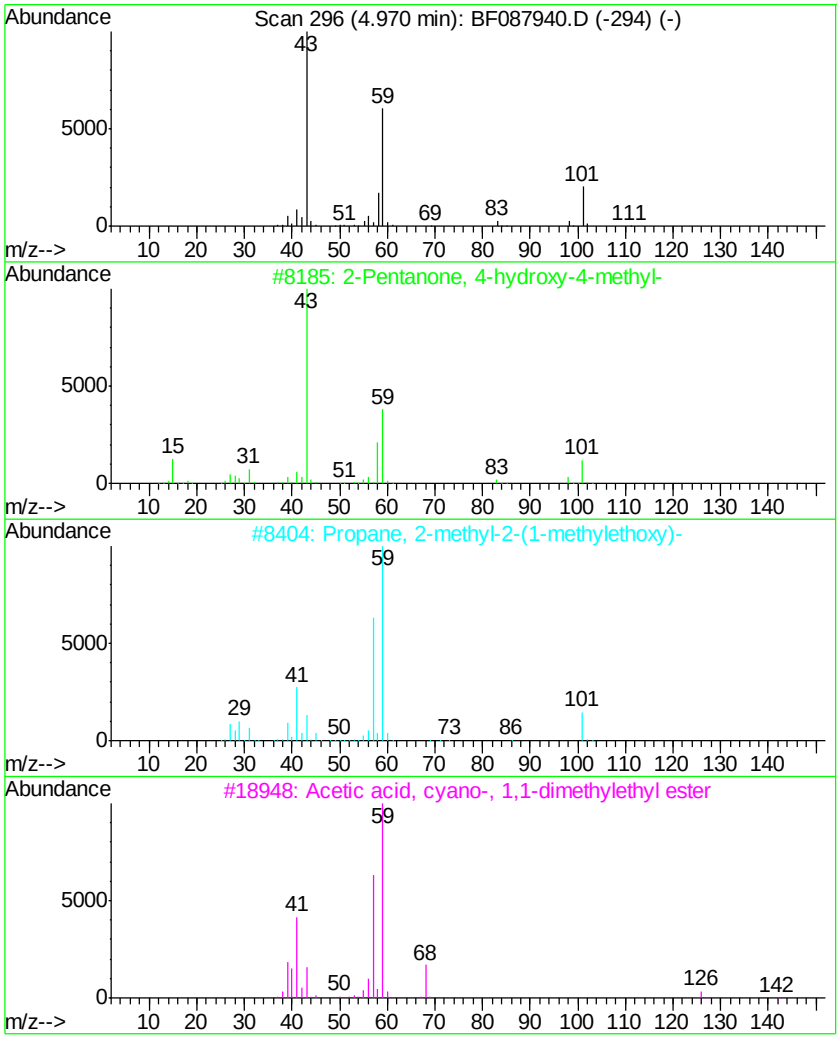
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

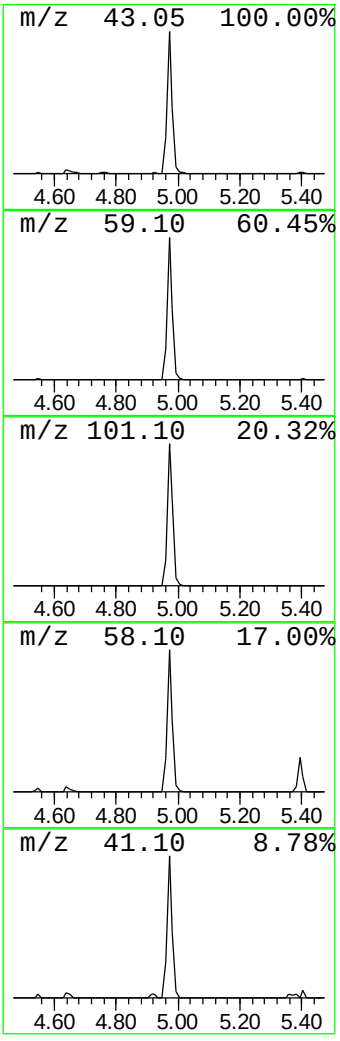
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	16.53 ng	506717	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

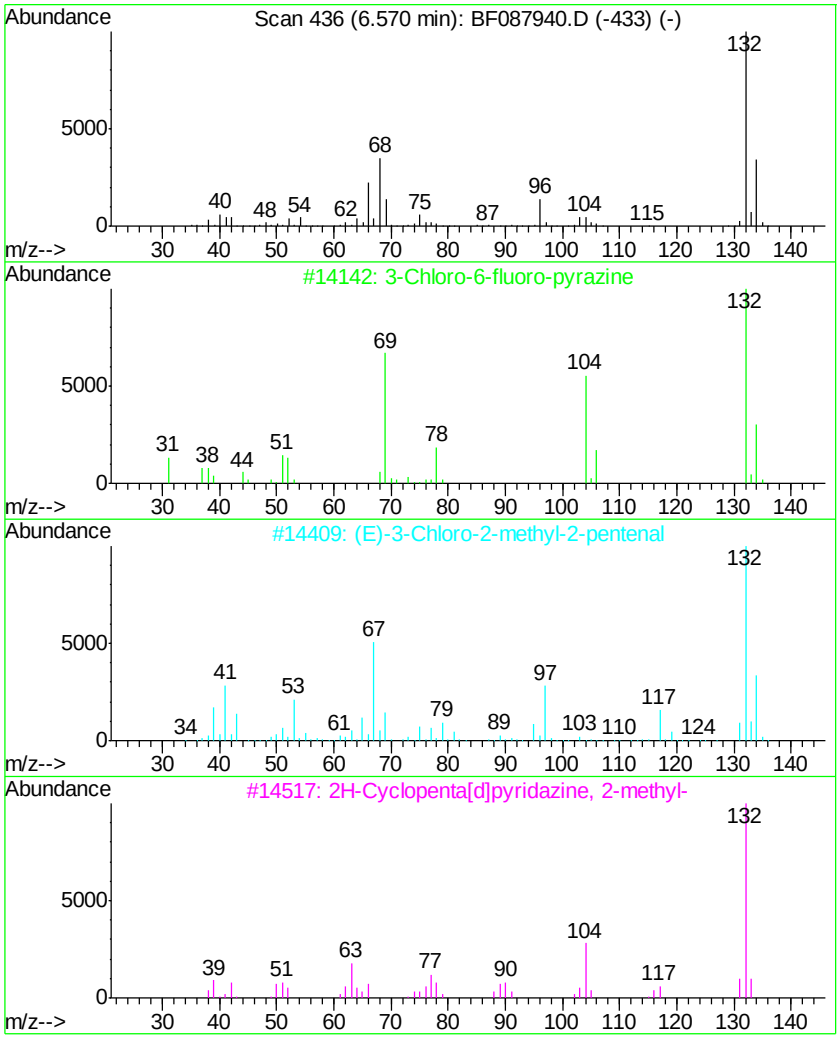
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

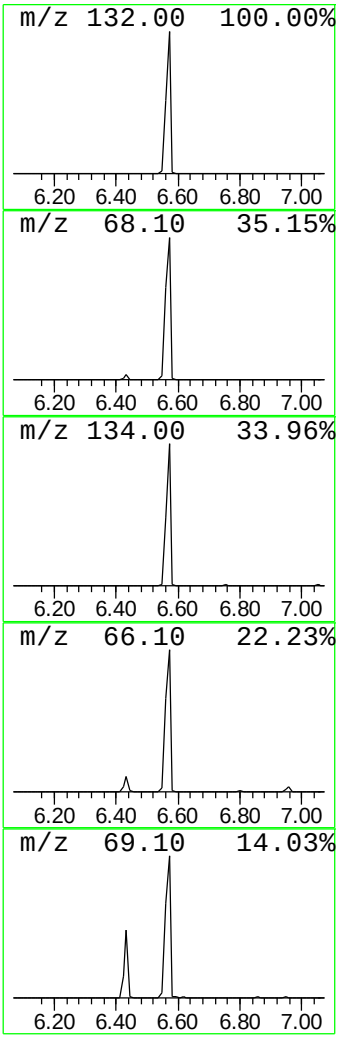
****

Peak Number 5 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	78.20 ng	2397670	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

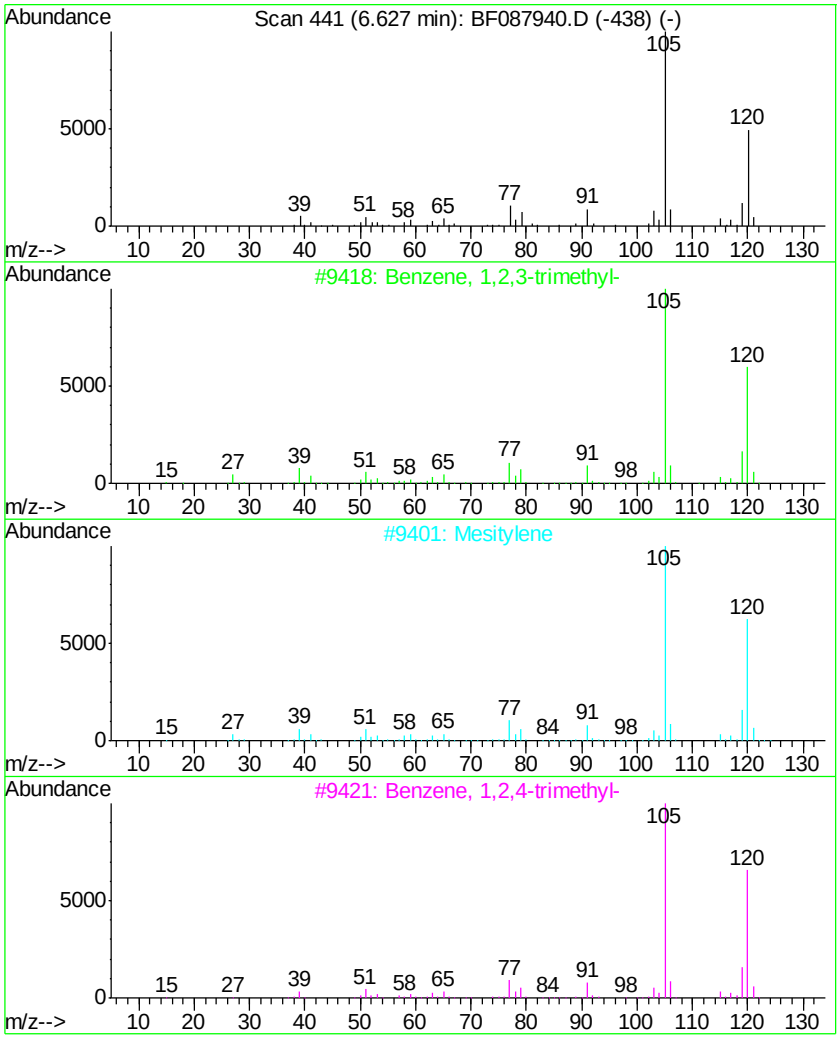
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

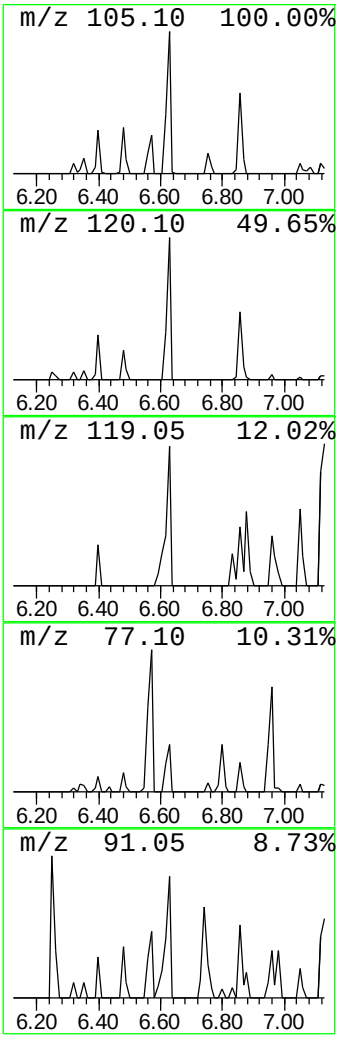
****

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	4.70 ng	144231	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2	Mesitylene	120	C9H12	000108-67-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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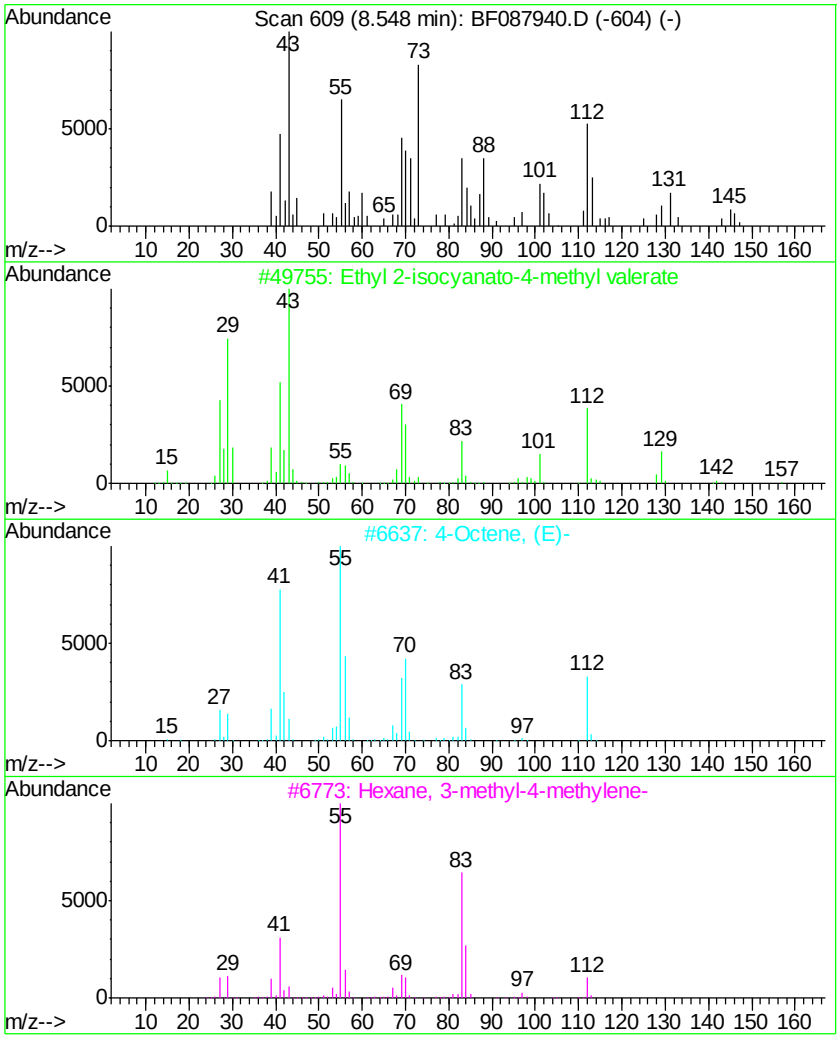
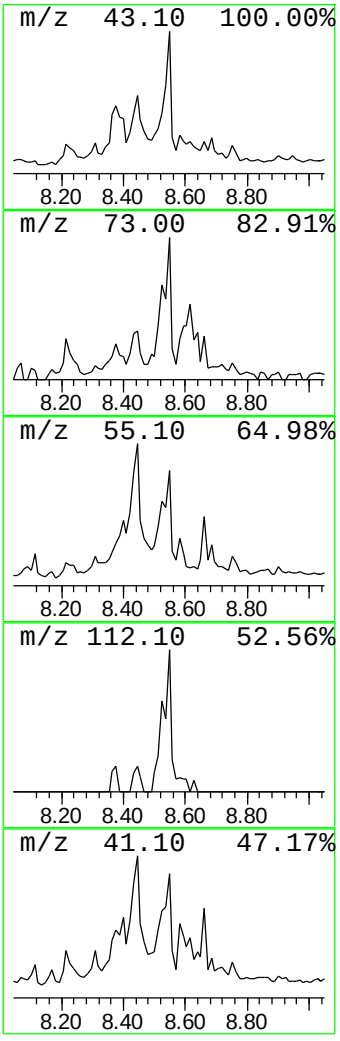
Peak Number 9 unknown8.55 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.55	3.18 ng	166958	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl 2-isocyanato-4-methyl vale...	185	C9H15NO3	064505-10-8	35
2	4-Octene, (E)-	112	C8H16	014850-23-8	27
3	Hexane, 3-methyl-4-methylene-	112	C8H16	003404-67-9	27
4	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	25
5	2-Butanol, 2-methyl-, acetate	130	C7H14O2	000625-16-1	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

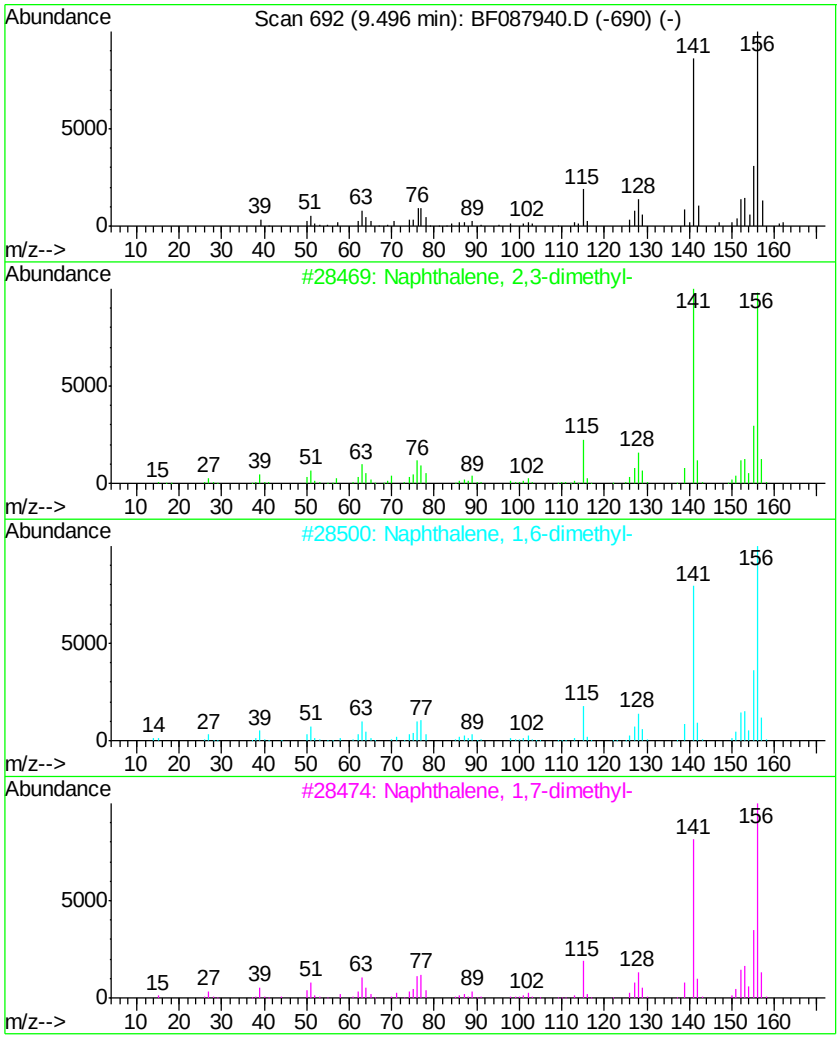
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

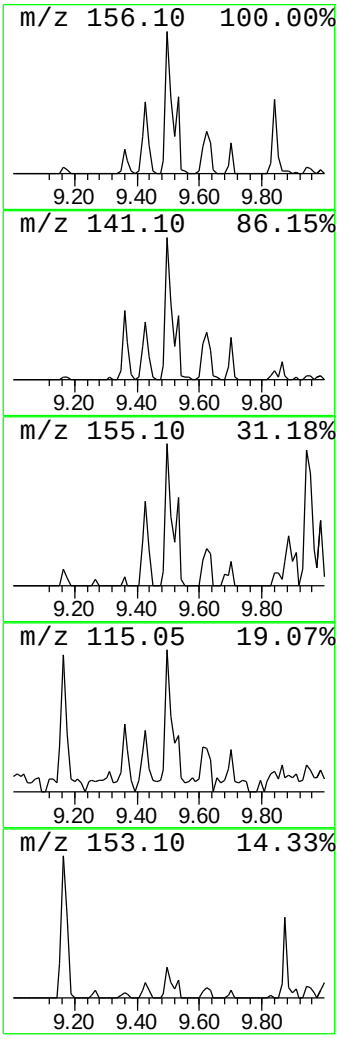
****

Peak Number 10 Naphthalene, 2,3-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	2.99 ng	143235	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	98
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	98
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
5	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	97





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061116\
Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

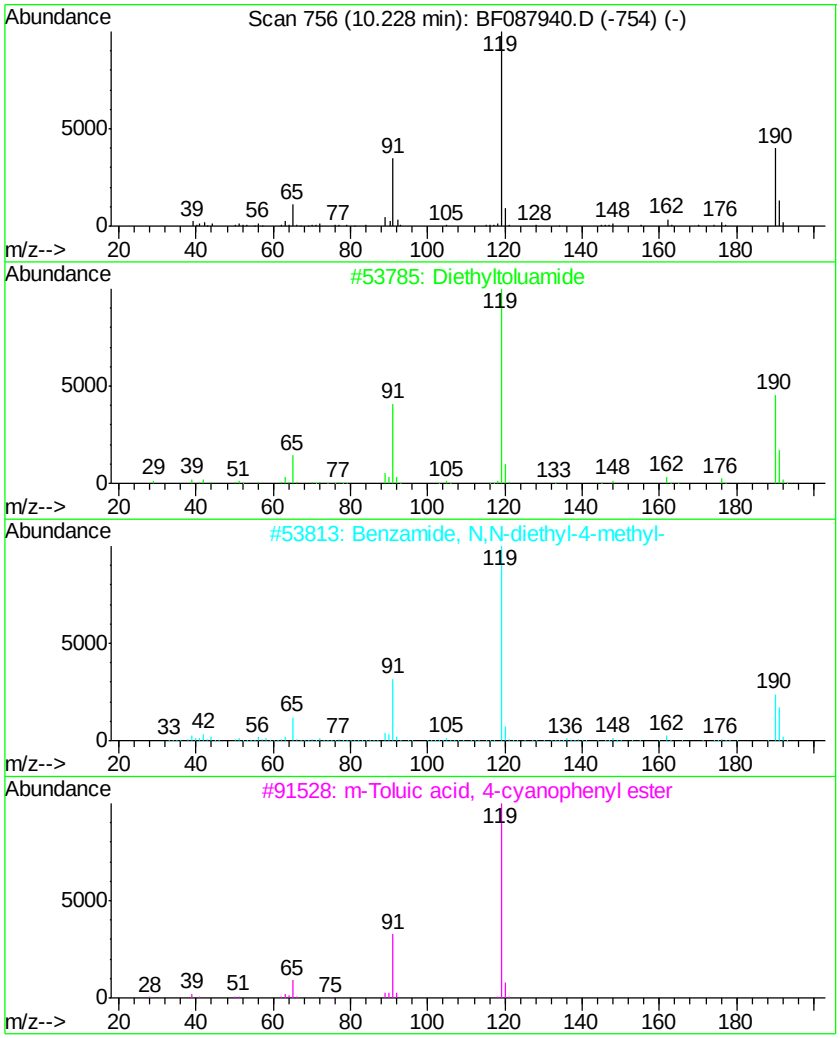
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

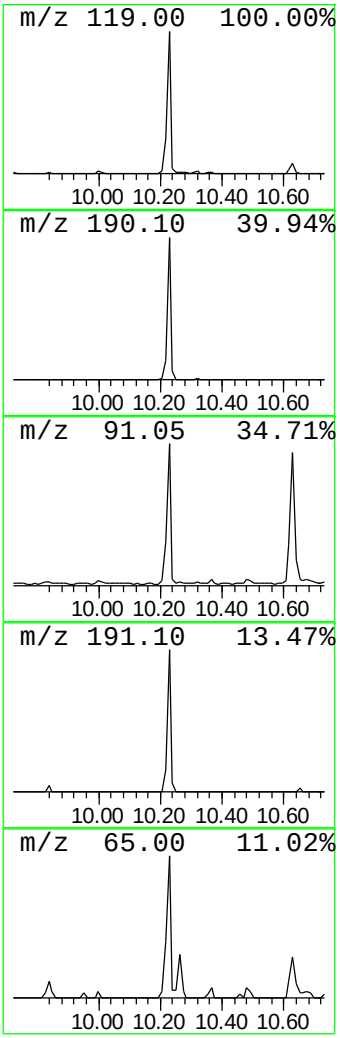
****

Peak Number 11 Diethyltoluamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.23	4.36 ng	208938	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	87
3	m-Toluic acid, 4-cyanophenyl ester	237	C15H11NO2	1000307-56-9	49
4	Benzoic acid, 4-methyl-, phenyl ...	212	C14H12O2	001900-85-2	47
5	Benzoic acid, 4-methyl-, [3-(4-m...	360	C23H20O4	306763-84-8	47





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Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

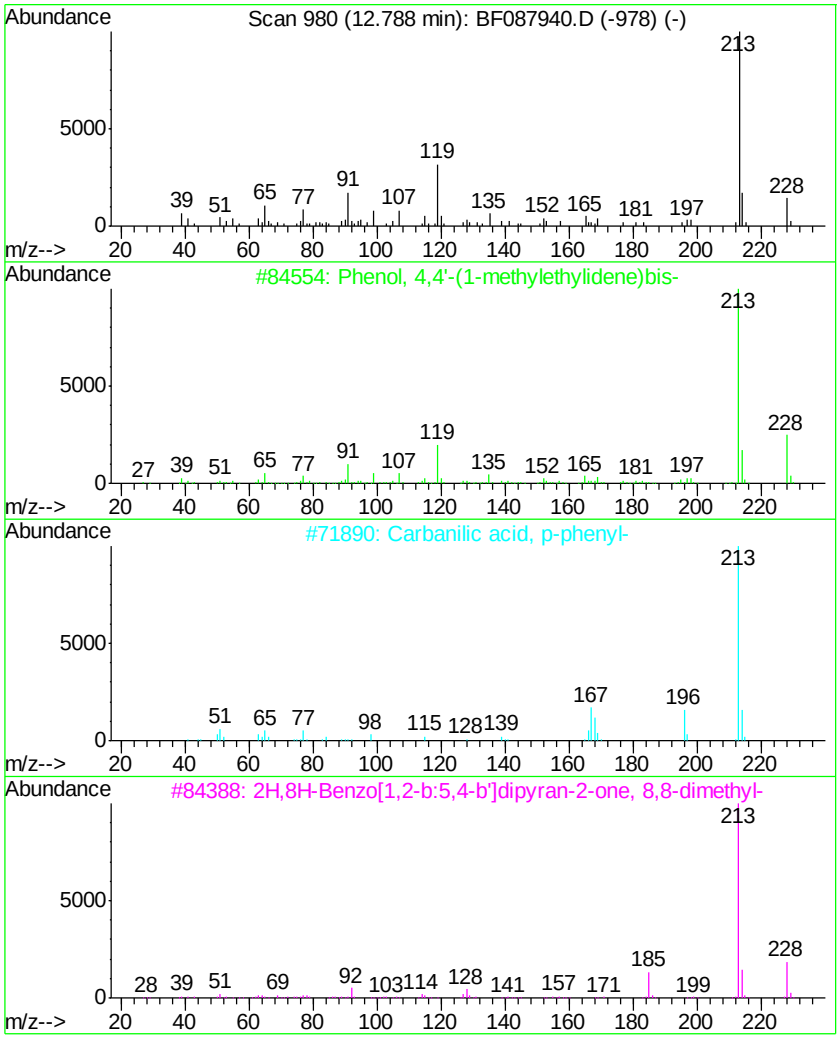
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

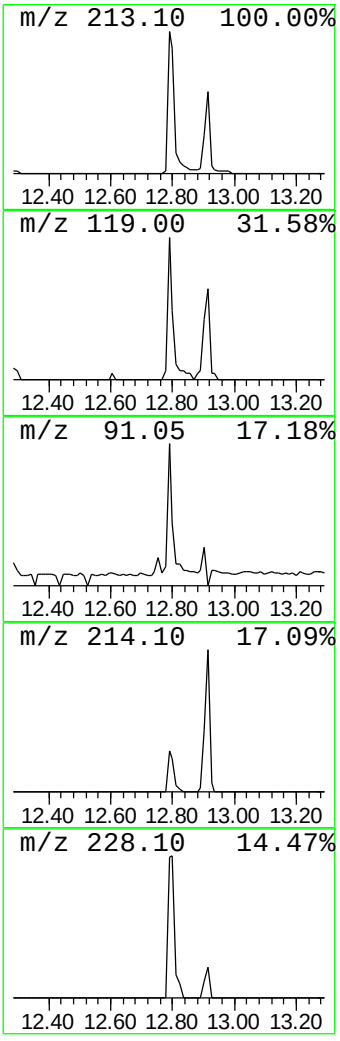
****

Peak Number 13 Phenol, 4,4'-(1-methylethyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	2.44 ng	107017	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	64
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	52
4	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	52
5	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061116\
Data File : BF087940.D
Acq On : 12 Jun 2016 10:44
Operator : UM/SJ
Sample : H3425-03
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP16-JMW0882

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	16.5	ng	506717	1	6.80	613230	20.0
unknown6.57	6.57	78.2	ng	2397670	1	6.80	613230	20.0
Benzene, 1,2,3-tr...	6.63	4.7	ng	144231	1	6.80	613230	20.0
unknown8.55	8.55	3.2	ng	166958	2	8.09	1049290	20.0
Naphthalene, 2,3-...	9.50	3.0	ng	143235	3	9.84	958955	20.0
Diethyltoluamide	10.23	4.4	ng	208938	3	9.84	958955	20.0
Phenol, 4,4'-(1-m...	12.79	2.4	ng	107017	5	13.95	877555	20.0