LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087692.D
Acq On : 5 Jun 2016 6:40
Operator : UM/SJ
Sample : H3344-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

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-BF060416.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	1.770	15	16	21	rVV	376470	469518	10.50%	1.229%
2	1.838	21	22	26	rVB	139812	157445	3.52%	0.412%
3	1.907	26	28	47	rVB	2360903	4472588	100.00%	11.703%
4	2.147	47	49	83	rVB	99501	495919	11.09%	1.298%
5	5.039	299	302	306	rBV	145394	182604	4.08%	0.478%
6	5.450	335	338	340	rBV	1855699	1736930	38.84%	4.545%
7	6.479	425	428	430	rBV	1344967	1225299	27.40%	3.206%
8	6.627	438	441	443	rBV	2827285	3277911	73.29%	8.577%
9	6.856	459	461	465	rBV	883352	772730	17.28%	2.022%
10	7.016	472	475	477	rBV	2924723	2823786	63.14%	7.389%
11	7.427	507	511	513	rVV	2205891	2711808	60.63%	7.096%
12	7.885	548	551	553	rBV2	27229	49658	1.11%	0.130%
13	7.942	553	556	558	rVB	43072	73658	1.65%	0.193%
14	8.147	571	574	576	rBV	906064	1115130	24.93%	2.918%
15	9.222	665	668	671	rBV	3142781	4295520	96.04%	11.240%
16	9.428	679	686	688	rVB	72569	107036	2.39%	0.280%
17	9.485	688	691	695	rBV	22383	47792	1.07%	0.125%
18	9.668	705	707	710	rBV2	51335	94253	2.11%	0.247%
19	9.759	713	715	717	rVB	86955	88266	1.97%	0.231%
20	9.896	724	727	729	rBV	1209782	1295332	28.96%	3.389%
21	9.931	729	730	732	rVB	1151990	827479	18.50%	2.165%
22	10.056	738	741	744	rBV3	31065	67099	1.50%	0.176%
23	10.319	760	764	765	rVV2	40310	64043	1.43%	0.168%
24	10.411	768	772	773	rBV2	57416	68245	1.53%	0.179%
25	10.433	773	774	777	rVB2	45205	64863	1.45%	0.170%
26	10.491	777	779	780	rBV	81062	102962	2.30%	0.269%
27	10.525	780	782	784	rVV	134869	222088	4.97%	0.581%
28	10.571	784	786	791	rVV3	74114	177760	3.97%	0.465%
29	10.685	793	796	798	rVV	2237820	2615180	58.47%	6.843%
30	10.811	802	807	811	rVB2	130100	231398	5.17%	0.605%
31	10.982	819	822	824	rBV	36270	76570	1.71%	0.200%
32	11.016	824	825	828	rVV	57730	55342	1.24%	0.145%
33	11.073	828	830	832	rVV2	49256	45696	1.02%	0.120%
34	11.165	837	838	842	rVB3	24156	45580	1.02%	0.119%

LSC Area Percent Report

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Acq On : 5 Jun 2016 6:40
Operator : UM/SJ
Sample : H3344-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

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-BF060416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.256	845	846	850	rVB2	43875	49867	1.11%	0.130%
36	11.382	854	857	859	rBV	1143906	1168945	26.14%	3.059%
37	11.485	865	866	873	rVB4	24560	49280	1.10%	0.129%
38	11.759	886	890	892	rBV3	33434	69514	1.55%	0.182%
39	11.862	897	899	901	rVV	48025	79474	1.78%	0.208%
40	11.908	901	903	905	rVV3	54752	87713	1.96%	0.230%
41	11.954	905	907	908	rVV	54195	75858	1.70%	0.198%
42	11.988	908	910	912	rVV	129469	167782	3.75%	0.439%
43	12.045	912	915	918	rVV	34373	69843	1.56%	0.183%
44	12.148	920	924	925	rVV3	30590	68068	1.52%	0.178%
45	12.308	936	938	942	rBV3	27370	78749	1.76%	0.206%
46	12.399	942	946	950	rVB3	27623	93039	2.08%	0.243%
47	12.582	961	962	964	rBV	49523	50503	1.13%	0.132%
48	12.697	970	972	975	rBV2	55382	73516	1.64%	0.192%
49	12.811	979	982	987	rVB2	113763	197595	4.42%	0.517%
50	12.971	993	996	998	rBV	3357105	3558651	79.57%	9.312%
51	13.017	998	1000	1003	rVV2	46535	64805	1.45%	0.170%
52	13.062	1003	1004	1006	rVV2	34825	49869	1.11%	0.130%
53	13.108	1006	1008	1013	rVB	95205	96512	2.16%	0.253%
54	13.519	1040	1044	1046	rBV	42416	69682	1.56%	0.182%
55	14.011	1084	1087	1089	rBV	1179123	1061739	23.74%	2.778%
56	15.440	1209	1212	1215	rBV	648862	777808	17.39%	2.035%

Sum of corrected areas: 38216300

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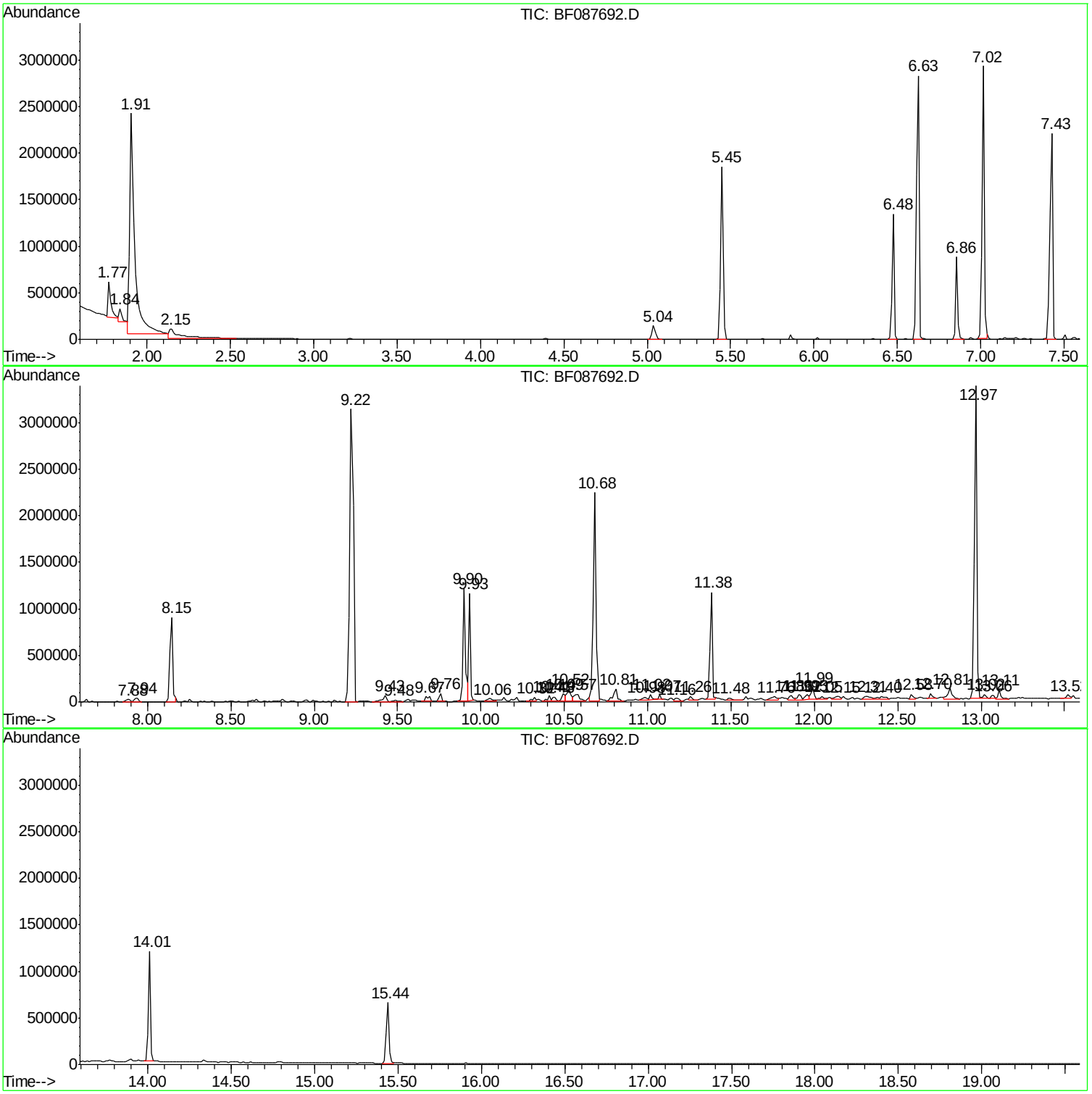
Operator : UM/SJ
Sample : H3344-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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\BF060416\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

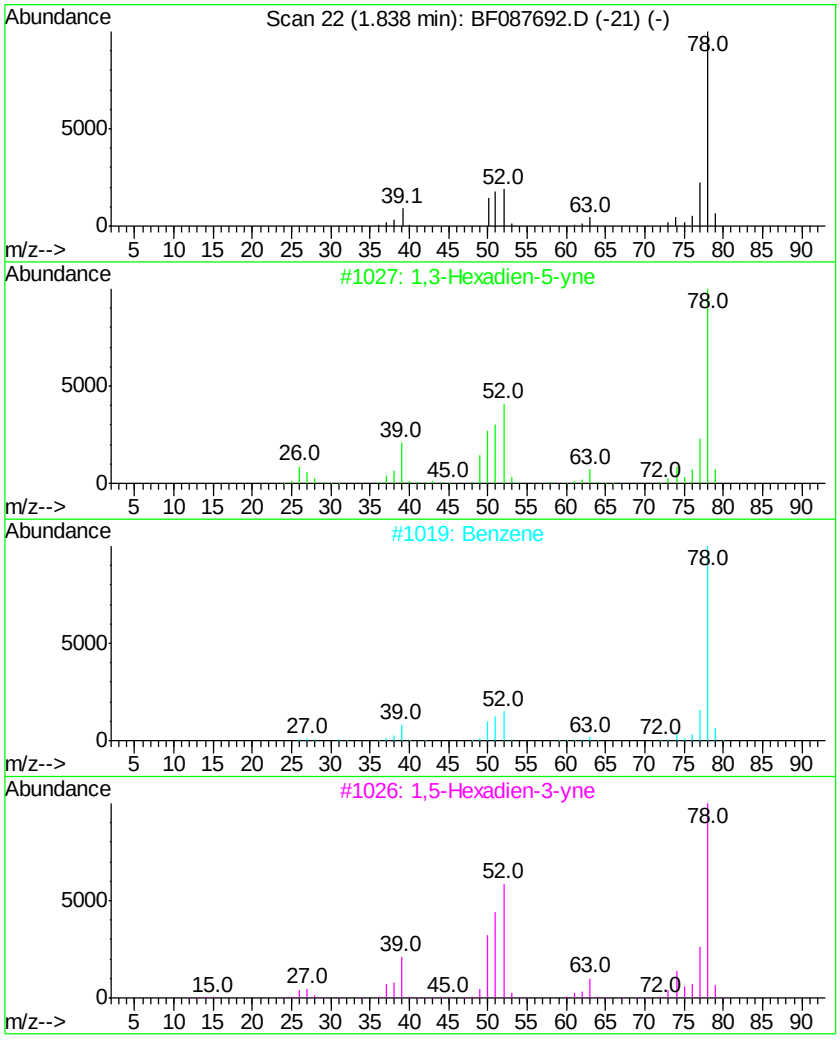
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

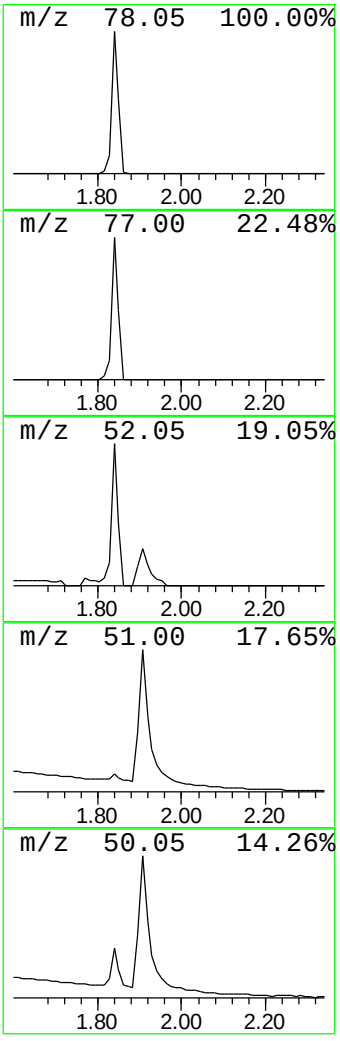
****

Peak Number 2 1,3-Hexadien-5-yne Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.84	4.08 ng	157445	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexadien-5-yne	78	C6H6	010420-90-3	91
2	Benzene	78	C6H6	000071-43-2	91
3	1,5-Hexadien-3-yne	78	C6H6	000821-08-9	83
4	6-Azidotetrazolo(b)pyridazine	162	C4H2N8	014393-79-4	64
5	Fumaronitrile	78	C4H2N2	000764-42-1	64





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Data File : BF087692.D
Acq On : 5 Jun 2016 6:40
Operator : UM/SJ
Sample : H3344-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

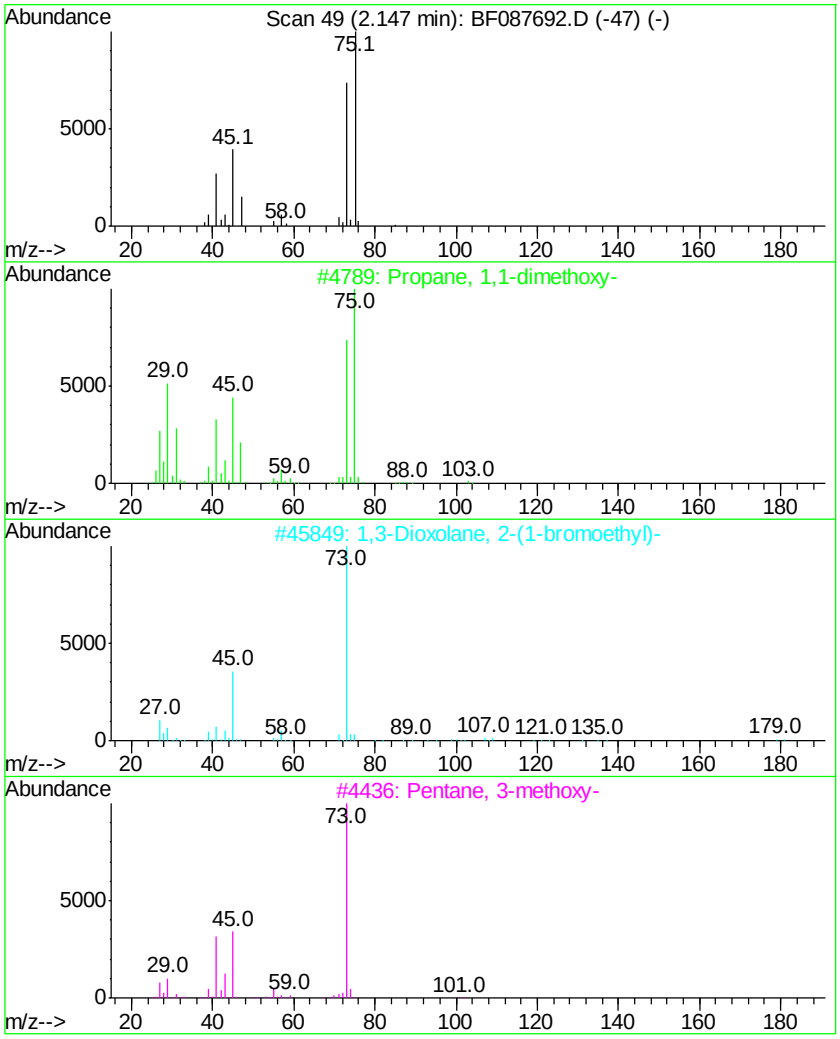
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

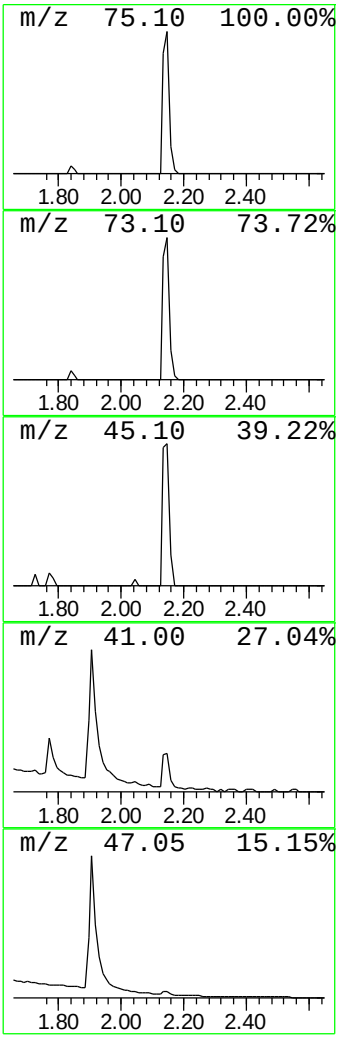
****

Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	12.84 ng	495919	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	25
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5	Glycine	75	C2H5NO2	000056-40-6	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087692.D
Acq On : 5 Jun 2016 6:40
Operator : UM/SJ
Sample : H3344-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

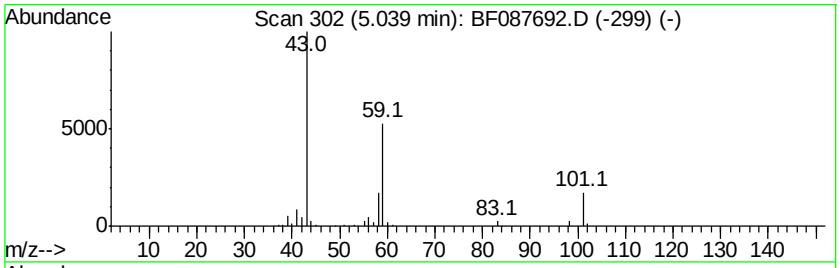
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

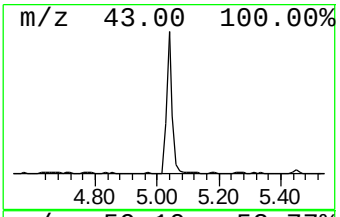
****

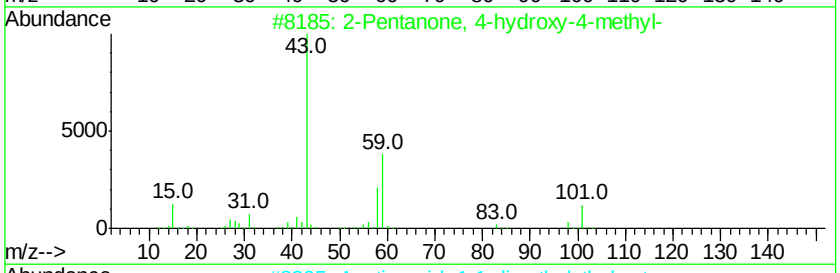
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

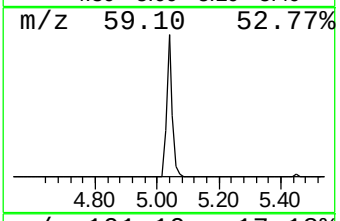
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	4.73 ng	182604	1,4-Dichlorobenzene-d4	6.86

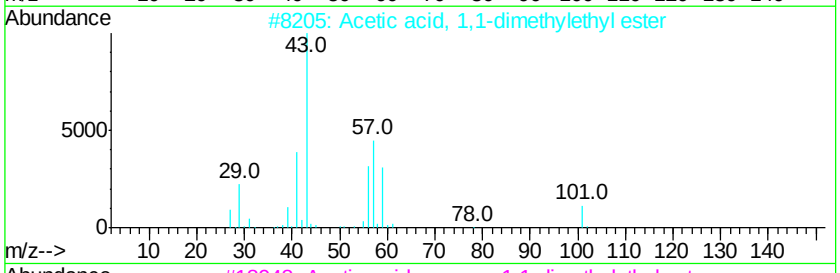
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	32
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10

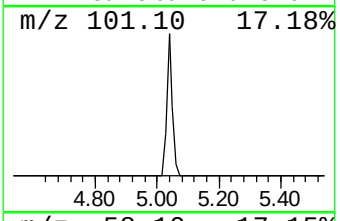


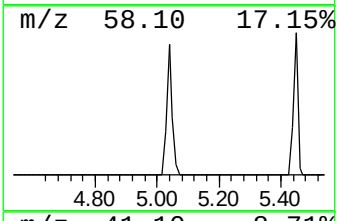


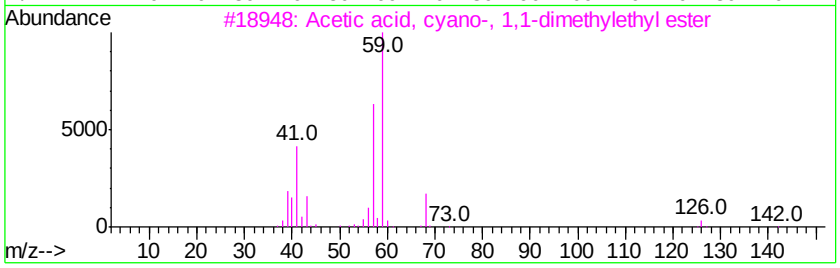


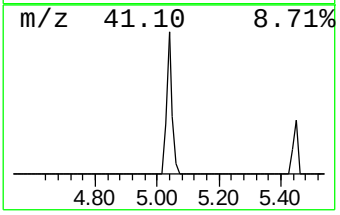












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Acq On : 5 Jun 2016 6:40
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Instrument : BNA_F
ClientSampleId : MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

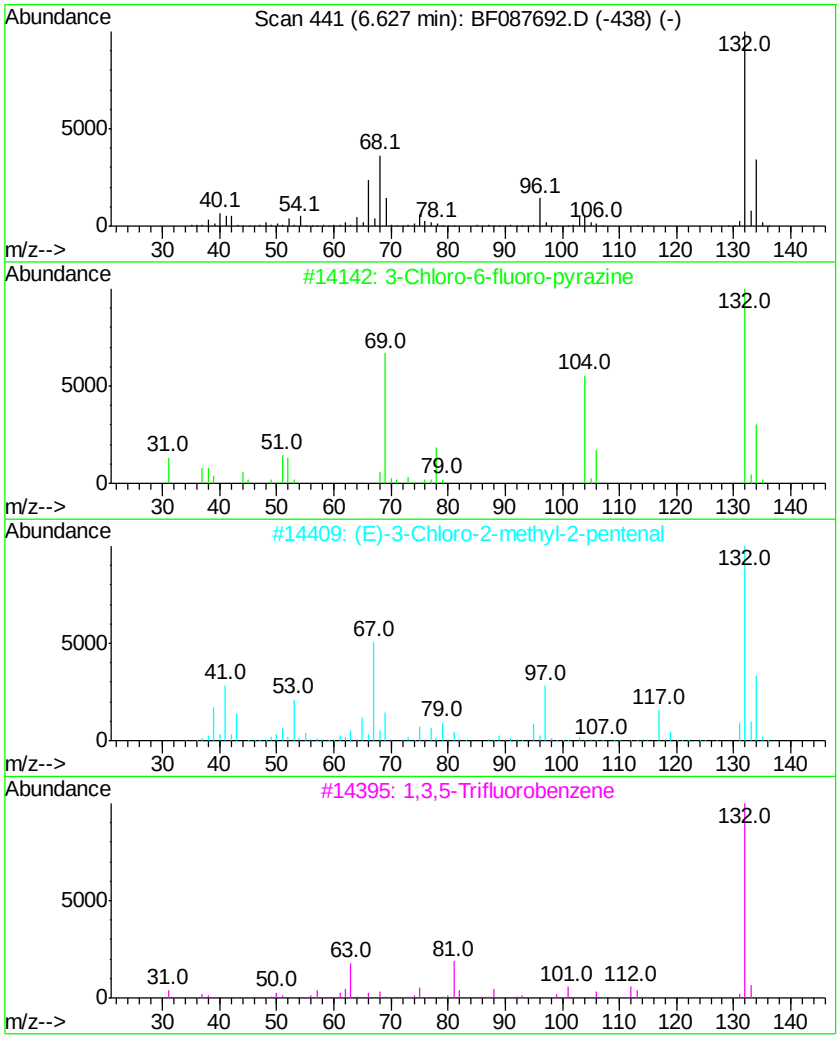
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

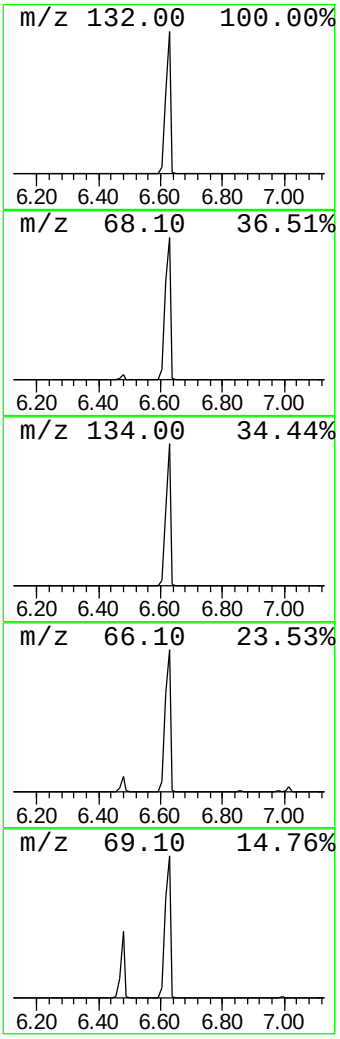
****

Peak Number 6 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	84.84 ng	3277910	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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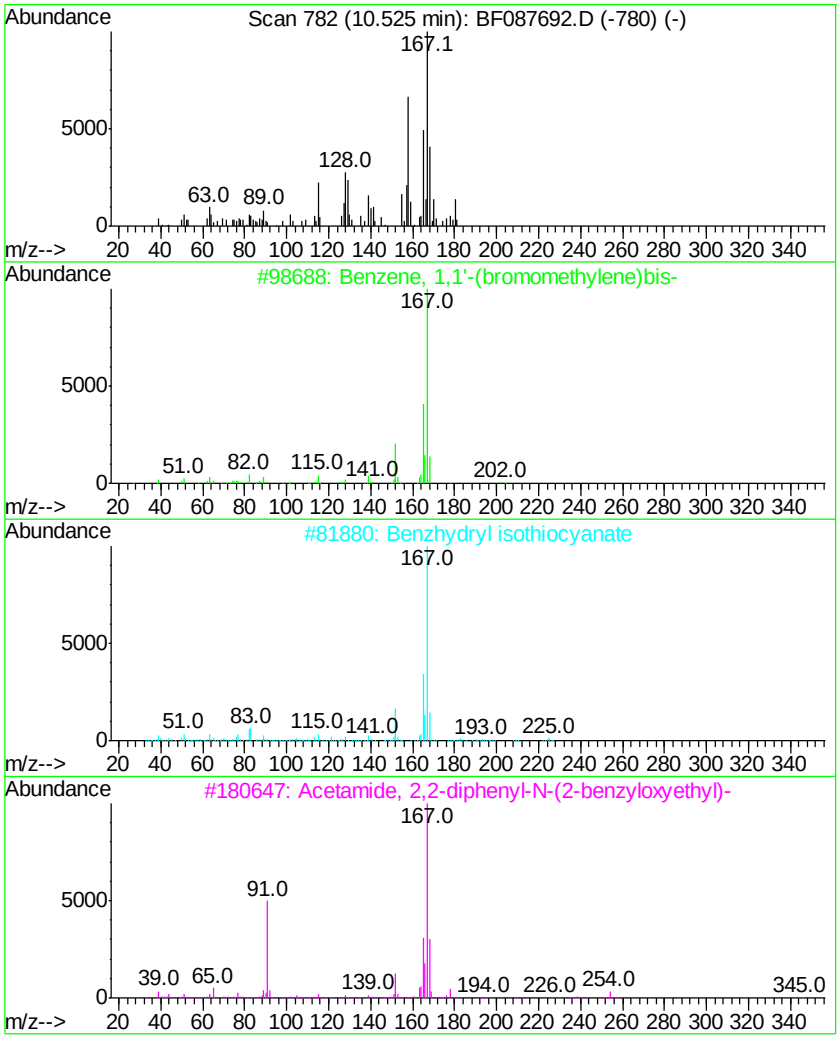
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

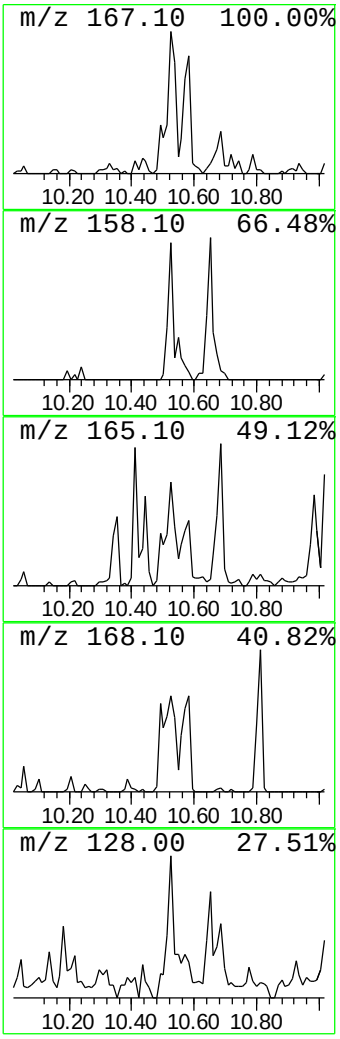
****

Peak Number 8 unknown10.52 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	3.43 ng	222088	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(bromomethylene)bis-	246	C13H11Br	000776-74-9	38
2	Benzhydryl isothiocyanate	225	C14H11NS	003550-21-8	38
3	Acetamide, 2,2-diphenyl-N-(2-ben...	345	C23H23NO2	329919-60-0	35
4	Carbazole	167	C12H9N	000086-74-8	22
5	1-Naphthalenol, 2-methyl-	158	C11H10O	007469-77-4	20





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Sample : H3344-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

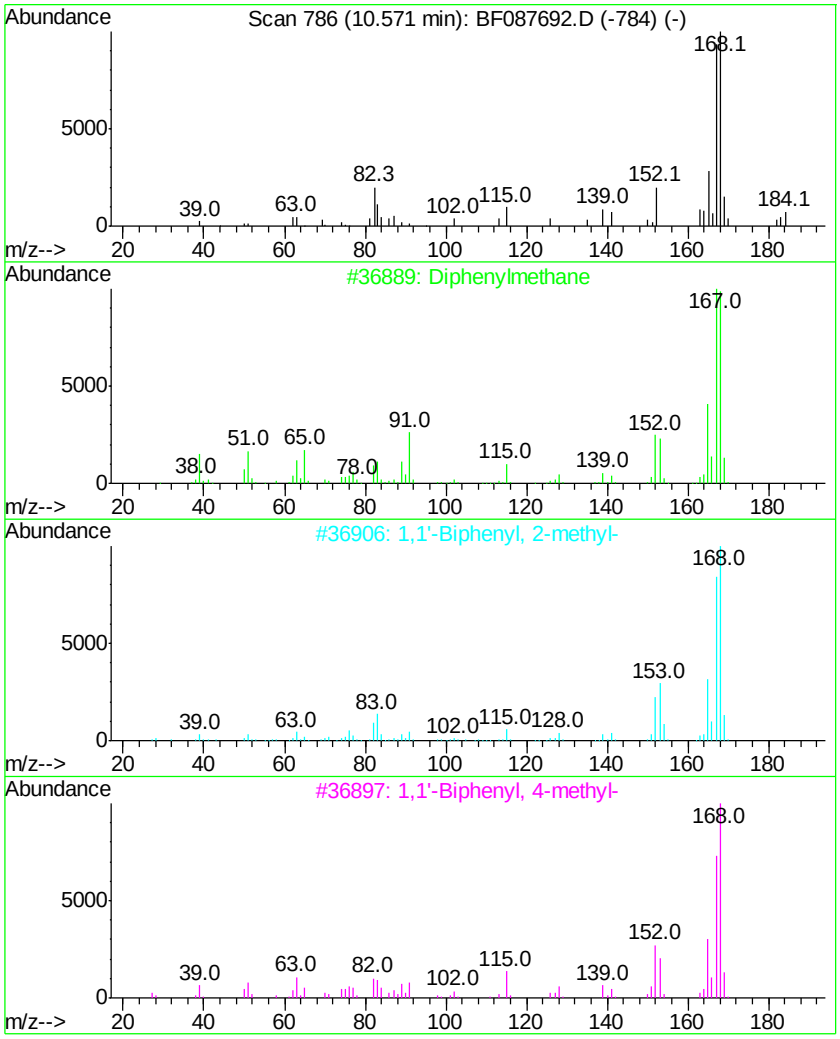
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

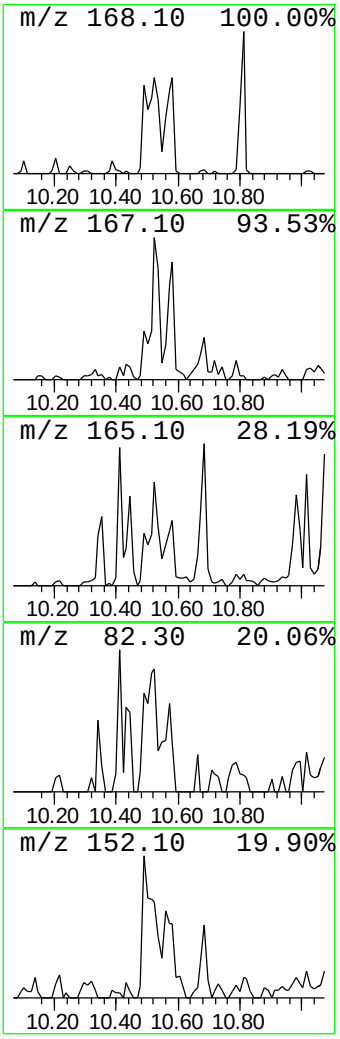
****

Peak Number 9 Diphenylmethane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	2.74 ng	177760	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diphenylmethane	168	C13H12	000101-81-5	76
2	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	64
3	1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	59
4	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	50
5	Thiazolo[3,2-c]pyrimidin-4-ium, ...	168	C7H8N2OS	024614-07-1	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087692.D
Acq On : 5 Jun 2016 6:40
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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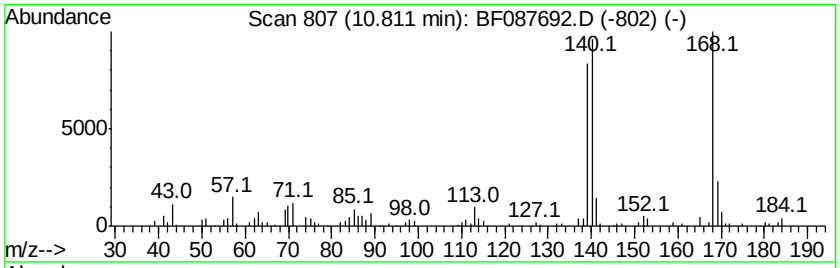
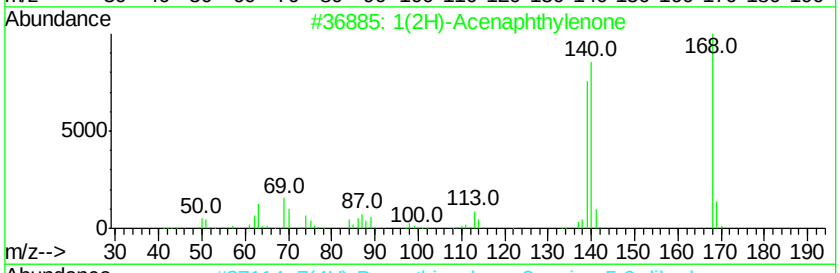
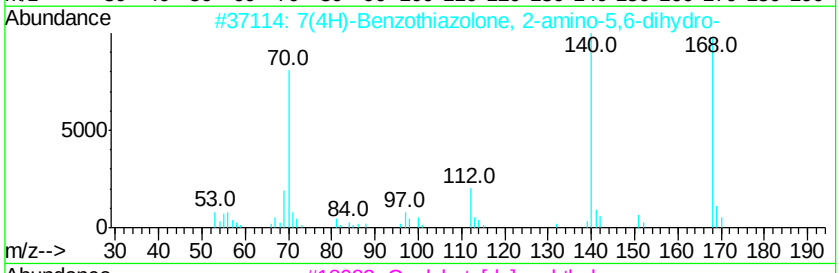
Peak Number 10 1(2H)-Acenaphthylenone Concentration Rank 8

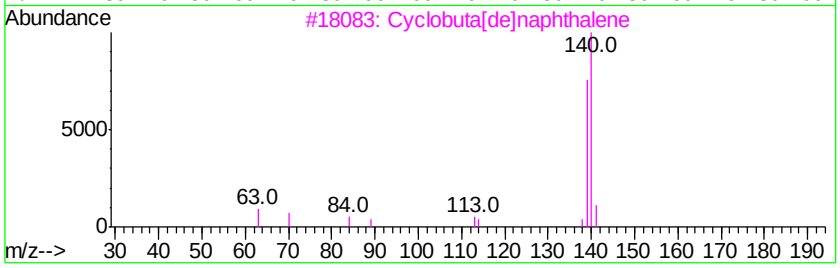
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.81	3.96 ng	231398	Phenanthrene-d10	11.38

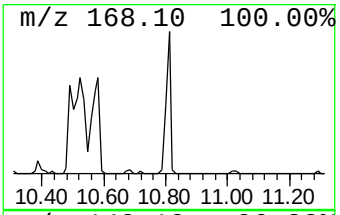
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	95
2	7(4H)-Benzothiazolone, 2-amino-5...	168	C7H8N2OS	017583-10-7	50
3	Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	49
4	Dibenzofuran	168	C12H8O	000132-64-9	47
5	Benzaldehyde, 2-fluoro-3-hydroxy-	140	C7H5FO2	103438-86-4	43

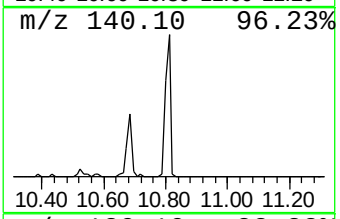


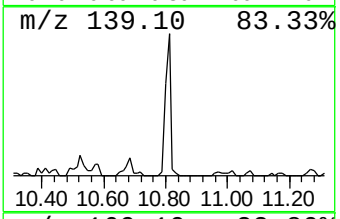


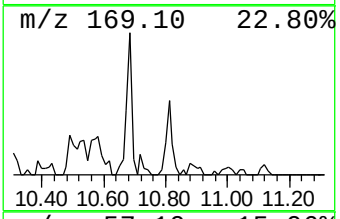


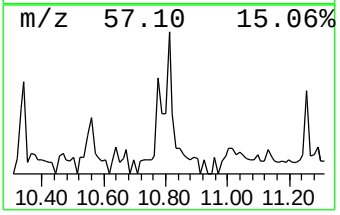












Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087692.D
Acq On : 5 Jun 2016 6:40
Operator : UM/SJ
Sample : H3344-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

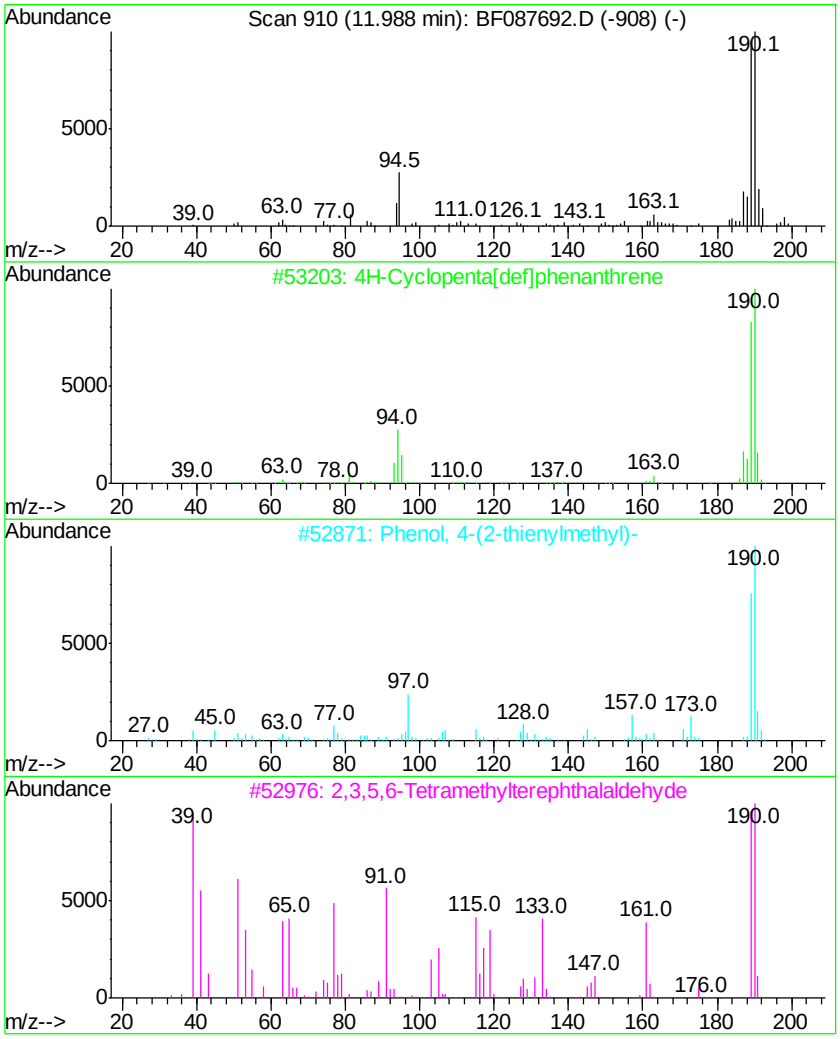
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

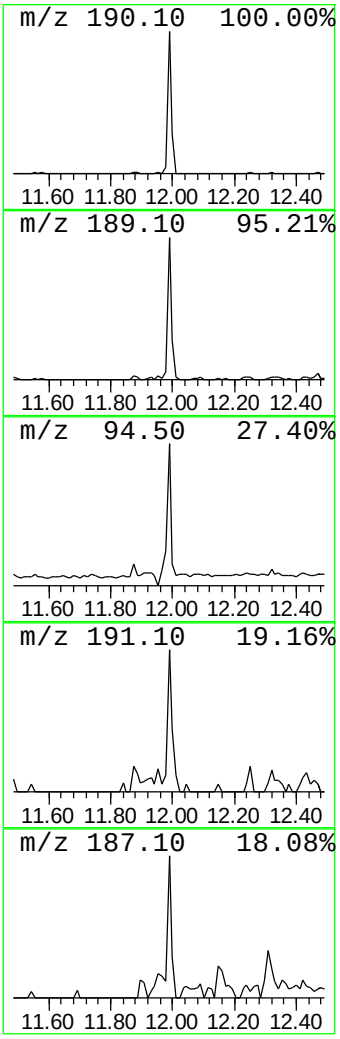
****

Peak Number 11 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.87 ng	167782	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	58
3	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087692.D
Acq On : 5 Jun 2016 6:40
Operator : UM/SJ
Sample : H3344-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-101

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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
1,3-Hexadien-5-yne	1.84	4.1	ng	157445	1	6.86	772730	20.0
Propane, 1,1-dime...	2.15	12.8	ng	495919	1	6.86	772730	20.0
2-Pentanone, 4-hy...	5.04	4.7	ng	182604	1	6.86	772730	20.0
unknown6.63	6.63	84.8	ng	3277910	1	6.86	772730	20.0
unknown10.52	10.52	3.4	ng	222088	3	9.90	1295330	20.0
Diphenylmethane	10.57	2.7	ng	177760	3	9.90	1295330	20.0
1(2H)-Acenaphthyl...	10.81	4.0	ng	231398	4	11.38	1168950	20.0
4H-Cyclopenta[def...	11.99	2.9	ng	167782	4	11.38	1168950	20.0