LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

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-BF042815.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	1.290	7	9	20	rVB	320496	831835	12.57%	2.849%
2	1.530	28	30	33	rVB	2299404	2434574	36.78%	8.338%
3	1.678	41	43	48	rVB	279739	374918	5.66%	1.284%
4	1.781	51	52	57	rVV	102317	219094	3.31%	0.750%
5	1.861	57	59	62	rVB	203061	267664	4.04%	0.917%
6	1.918	62	64	104	rVB	3515554	6619829	100.00%	22.673%
7	5.187	349	350	357	rVB	83893	112864	1.70%	0.387%
8	5.679	390	393	395	rBV	652468	727317	10.99%	2.491%
9	6.925	500	502	504	rBV	1041467	928431	14.02%	3.180%
10	7.085	514	516	519	rBV	653267	817887	12.36%	2.801%
11	7.382	540	542	544	rBV	491780	445484	6.73%	1.526%
12	7.565	556	558	561	rVB	465587	578378	8.74%	1.981%
13	8.068	600	602	605	rBV	563826	516054	7.80%	1.767%
14	8.959	678	680	683	rBV	733447	632408	9.55%	2.166%
15	10.308	795	798	800	rBV	1708726	1516466	22.91%	5.194%
16	11.142	868	871	873	rBV	618924	695036	10.50%	2.380%
17	12.114	954	956	959	rBV	995769	1121596	16.94%	3.841%
18	12.982	1030	1032	1034	rBV	679475	839219	12.68%	2.874%
19	13.017	1034	1035	1037	rVB	533031	399218	6.03%	1.367%
20	13.074	1037	1040	1042	rBV	53478	77503	1.17%	0.265%
21	13.611	1085	1087	1089	rBV	75633	94719	1.43%	0.324%
22	13.645	1089	1090	1092	rVV	99277	109445	1.65%	0.375%
23	13.691	1092	1094	1097	rVV2	47986	76784	1.16%	0.263%
24	13.748	1097	1099	1101	rVV	103545	131657	1.99%	0.451%
25	14.011	1119	1122	1125	rBV	71974	117782	1.78%	0.403%
26	14.400	1153	1156	1160	rVB3	63305	94662	1.43%	0.324%
27	14.491	1162	1164	1166	rBV	473973	579119	8.75%	1.983%
28	14.674	1177	1180	1182	rBV3	41128	76563	1.16%	0.262%
29	14.777	1186	1189	1192	rVV	697193	764785	11.55%	2.619%
30	14.845	1193	1195	1199	rVB2	40252	75358	1.14%	0.258%
31	14.982	1204	1207	1210	rVB	2265780	2215298	33.46%	7.587%
32	15.062	1210	1214	1216	rBV3	46513	76352	1.15%	0.262%
33	15.177	1220	1224	1227	rVV3	34701	91743	1.39%	0.314%
34	15.325	1235	1237	1239	rBV	64842	83320	1.26%	0.285%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

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-BF042815.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.600	1256	1261	1262	rBV4	30526	72384	1.09%	0.248%
36	15.817	1278	1280	1283	rBV	65442	95709	1.45%	0.328%
37	15.954	1290	1292	1295	rBV2	54600	109945	1.66%	0.377%
38	16.000	1295	1296	1299	rBV2	36161	76180	1.15%	0.261%
39	16.148	1307	1309	1314	rBV2	158331	269775	4.08%	0.924%
40	16.274	1317	1320	1322	rBV2	815047	1233642	18.64%	4.225%
41	16.766	1361	1363	1365	rVV	66416	109001	1.65%	0.373%
42	17.543	1428	1431	1436	rBV	219256	472279	7.13%	1.618%
43	17.863	1456	1459	1461	rBV	159575	205866	3.11%	0.705%
44	17.920	1462	1464	1468	rVB	186331	296792	4.48%	1.016%
45	18.000	1468	1471	1473	rBV	572933	902603	13.63%	3.091%
46	19.497	1600	1602	1608	rBV2	83276	212532	3.21%	0.728%
47	19.954	1639	1642	1655	rVB	116857	397524	6.01%	1.361%

Sum of corrected areas: 29197594

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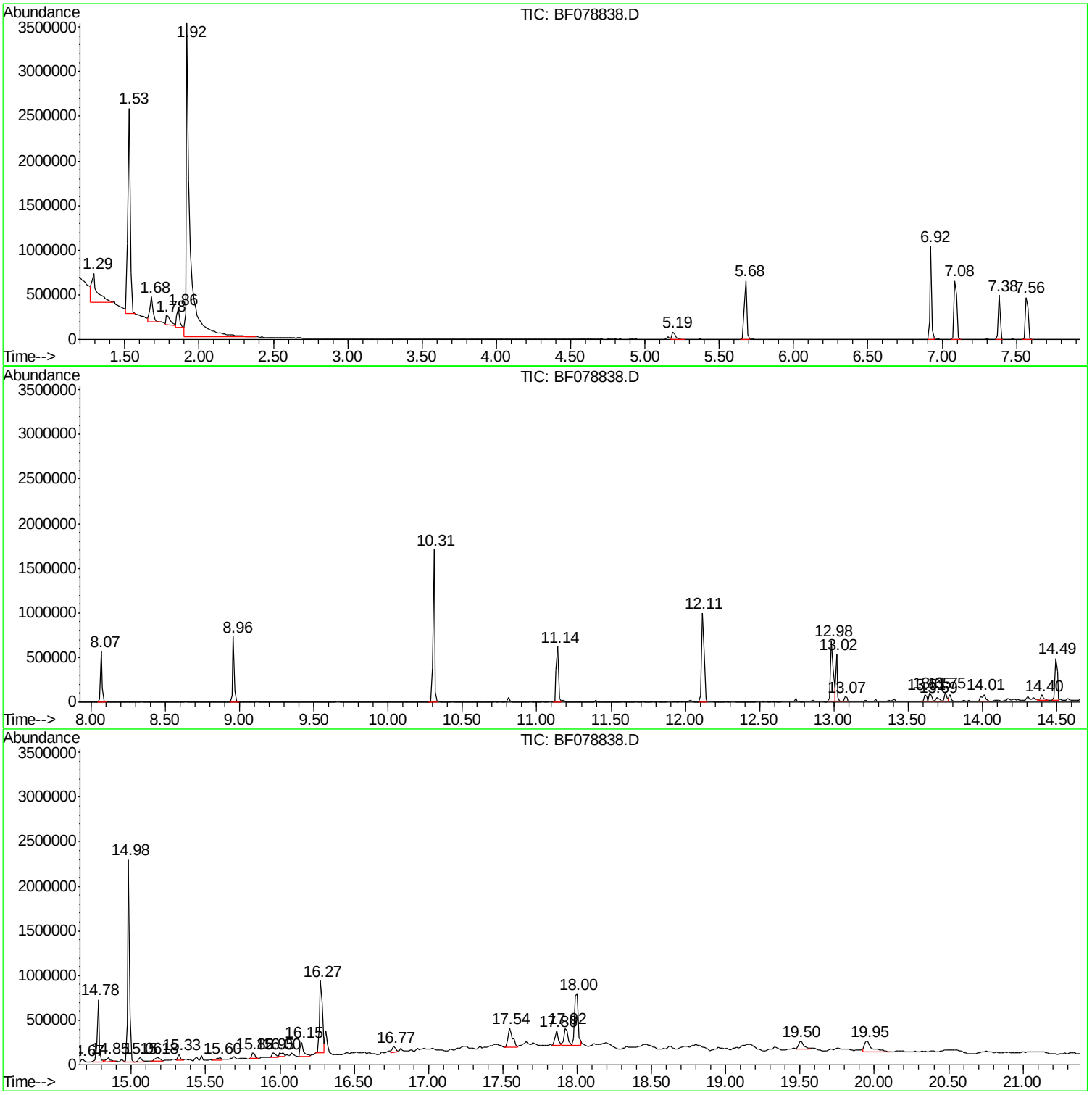
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

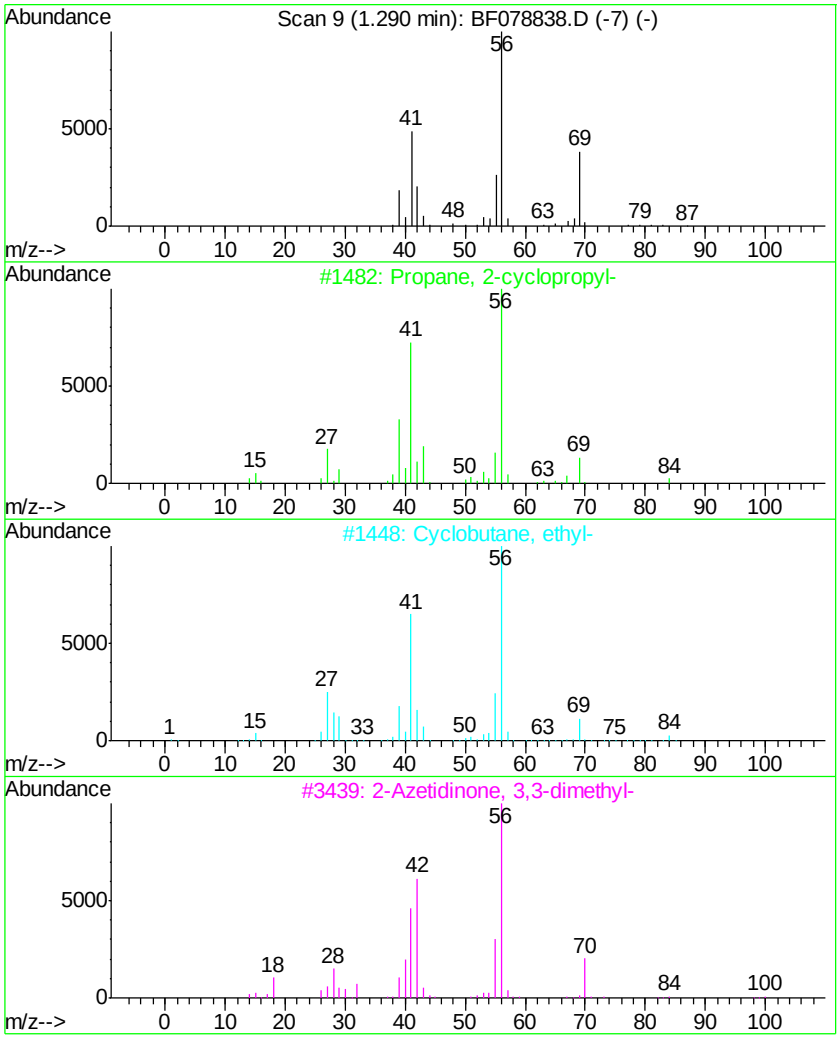
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

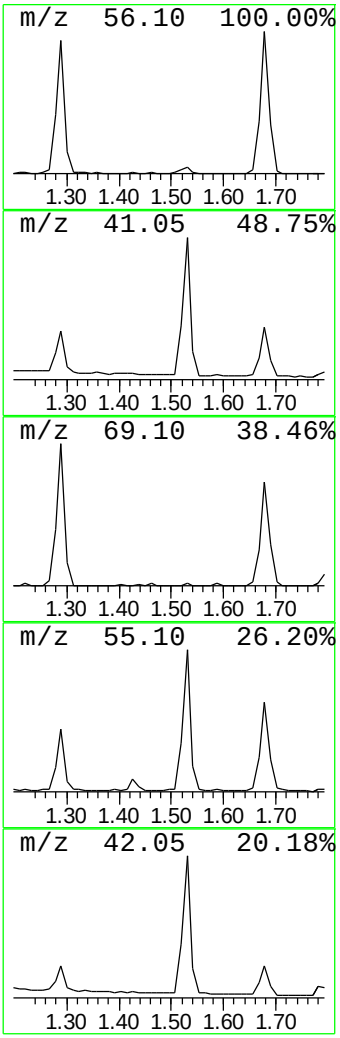
****

Peak Number 1 unknown1.29 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.29	37.35 ng	831835	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9
3	2-Azetidinone, 3,3-dimethyl-	99	C5H9NO	007486-91-1	9
4	Aziridine, 1-(2-buten-2-yl)-	97	C6H11N	1000158-95-2	9
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

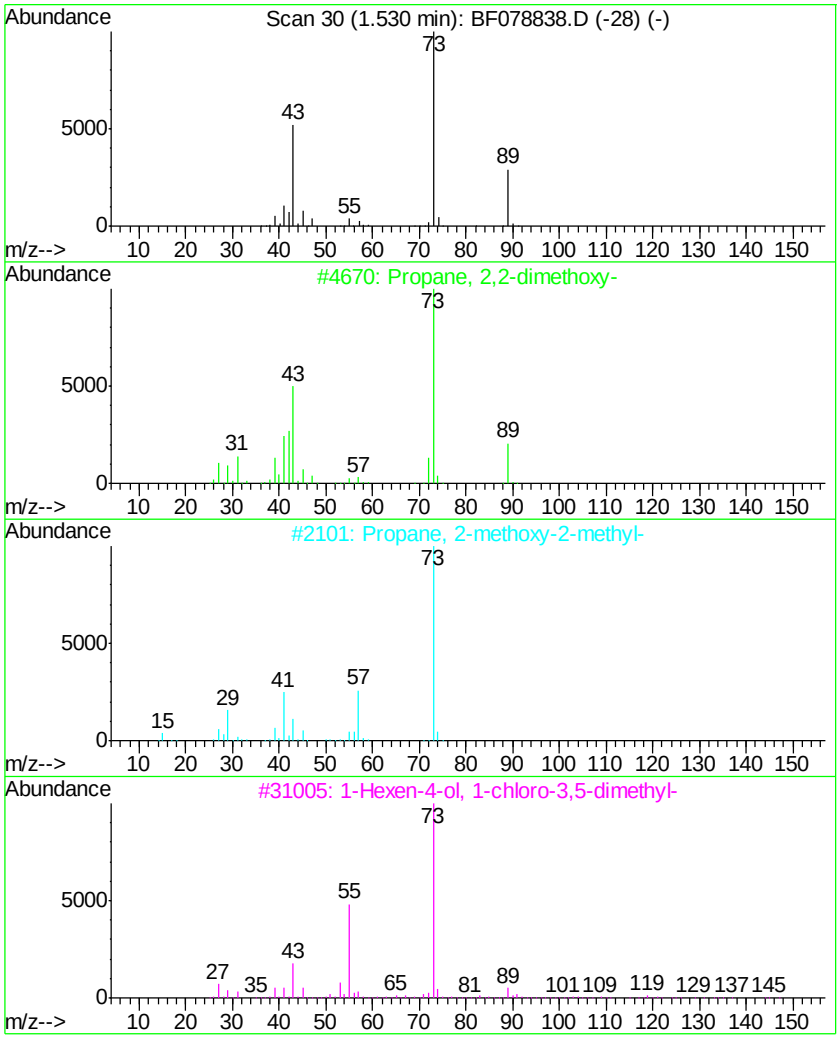
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

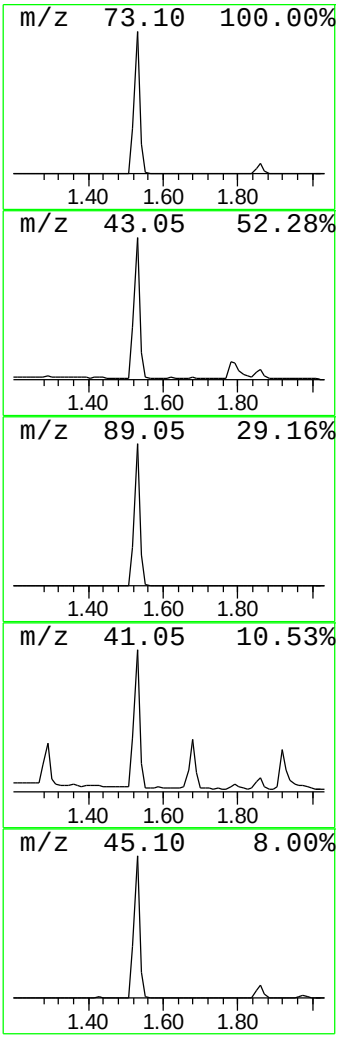
****

Peak Number 2 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.53	109.30 ng	2434570	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

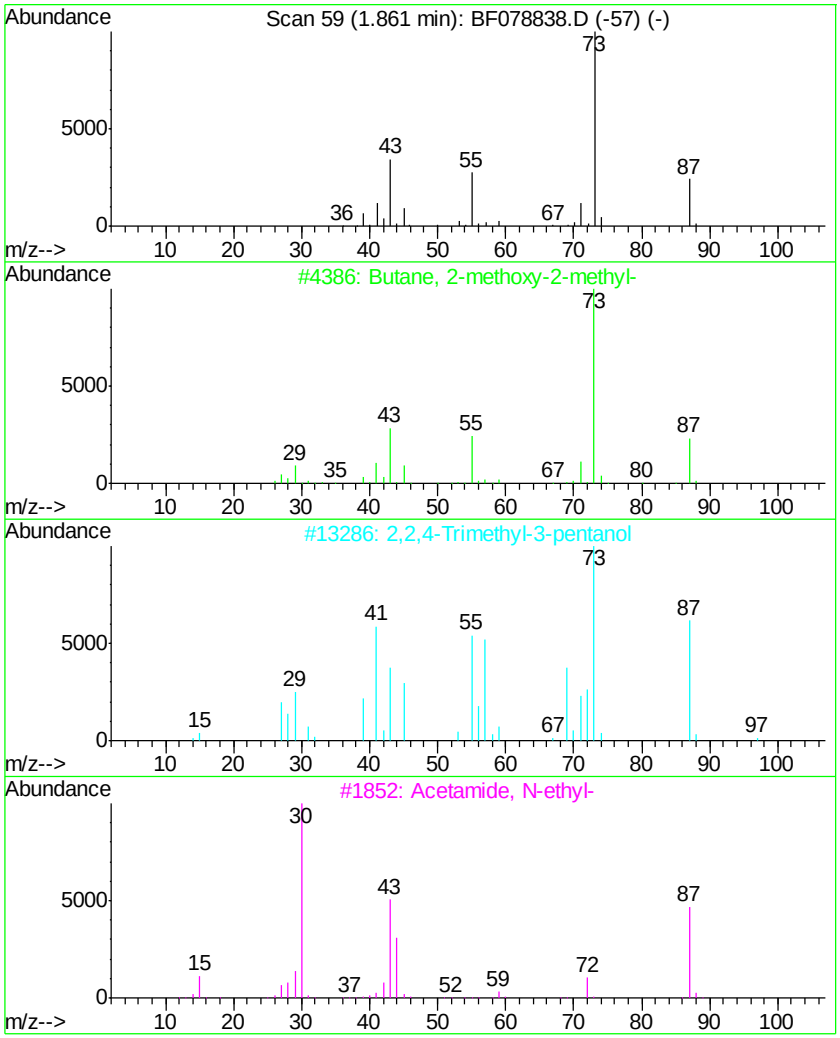
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

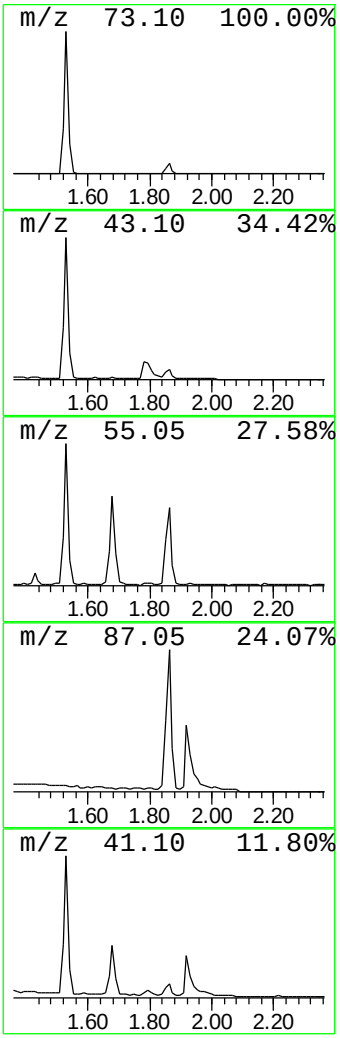
****

Peak Number 5 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.86	12.02 ng	267664	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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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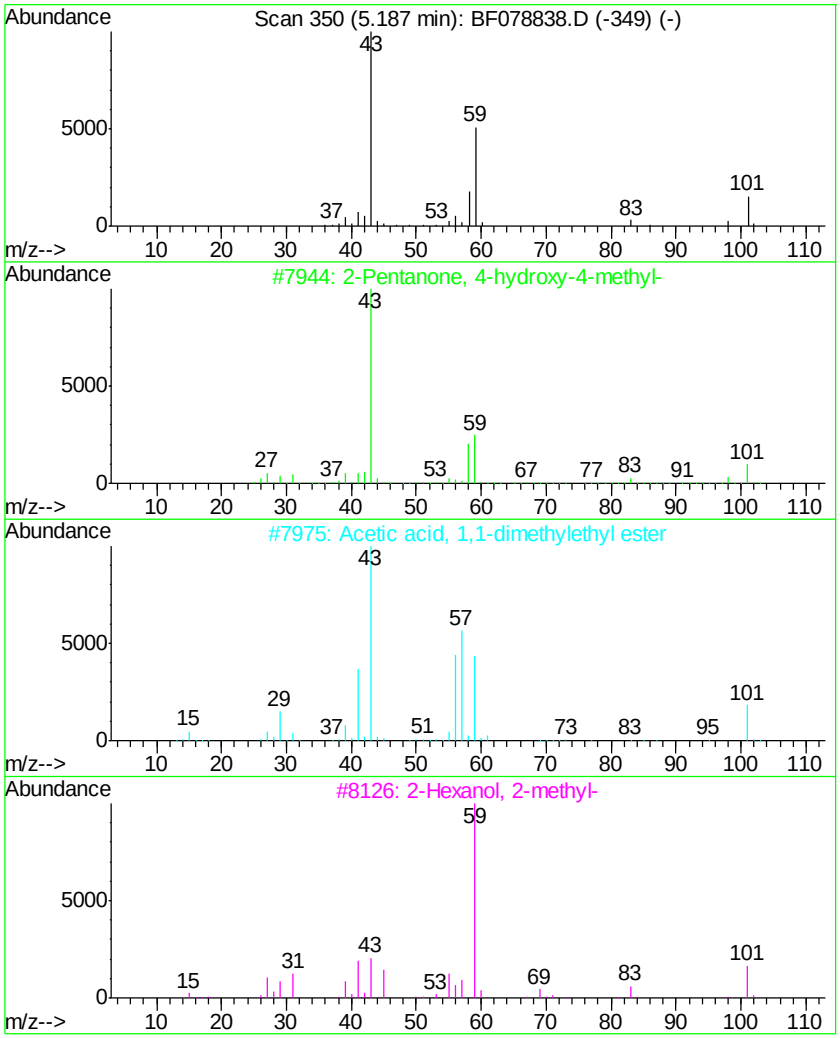
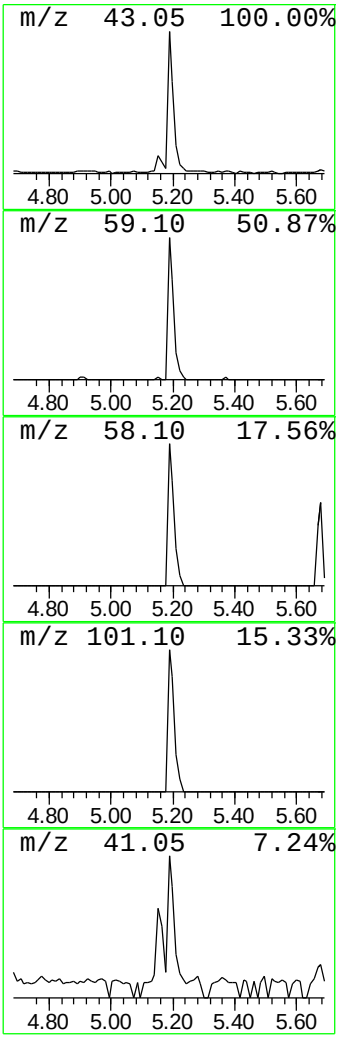
Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	5.07 ng	112864	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

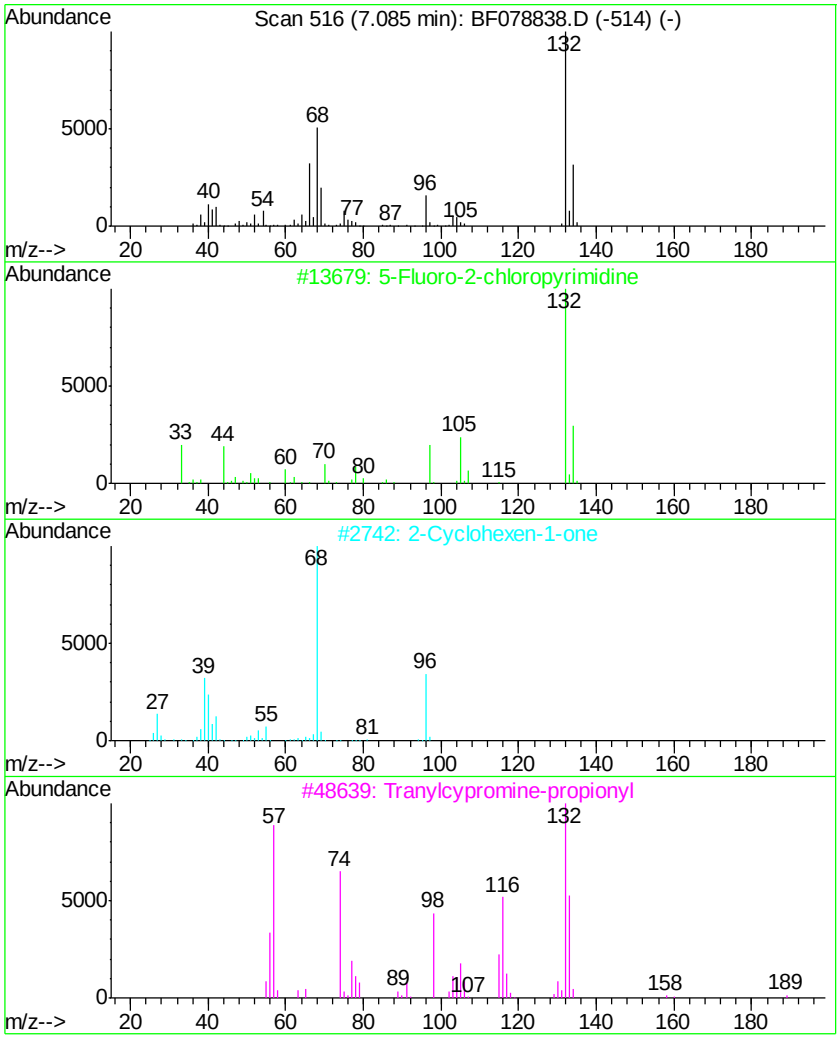
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

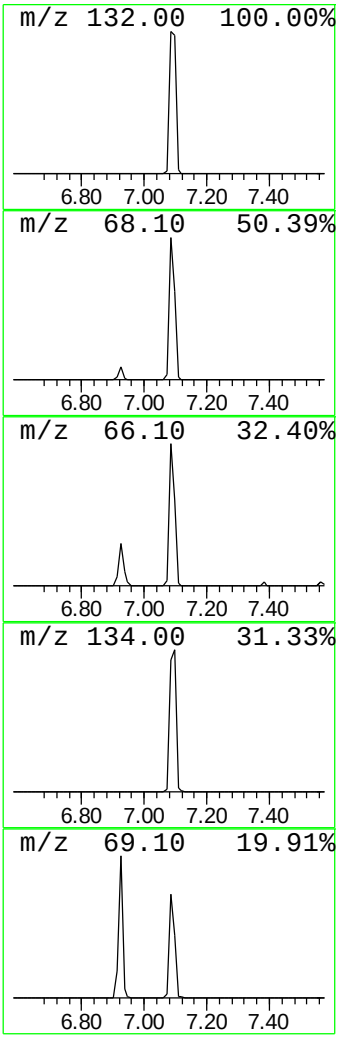
****

Peak Number 8 unknown7.08 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	36.72 ng	817887	1,4-Dichlorobenzene-d4	7.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

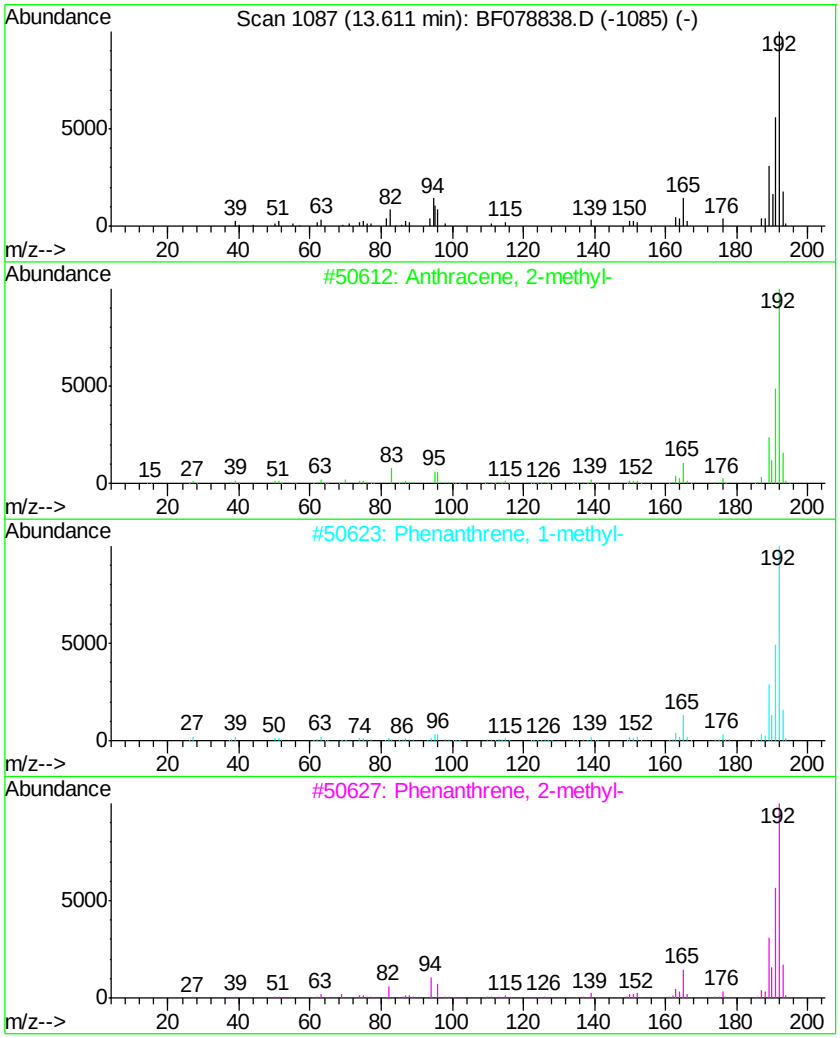
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

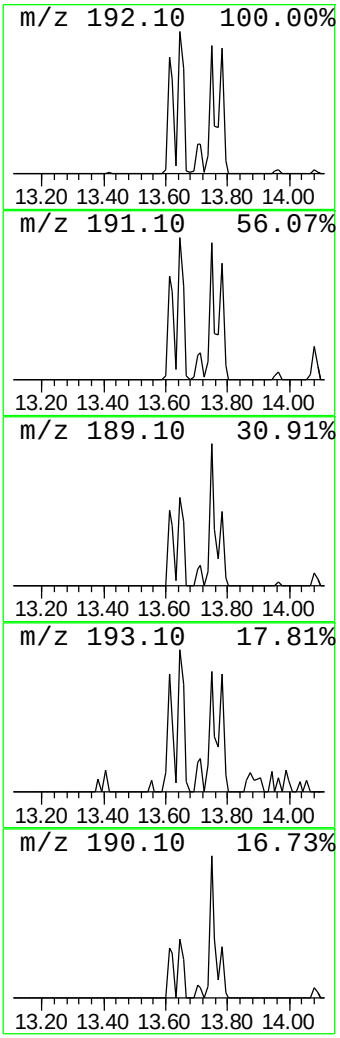
****

Peak Number 10 Anthracene, 2-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	2.26 ng	94719	Phenanthrene-d10	12.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

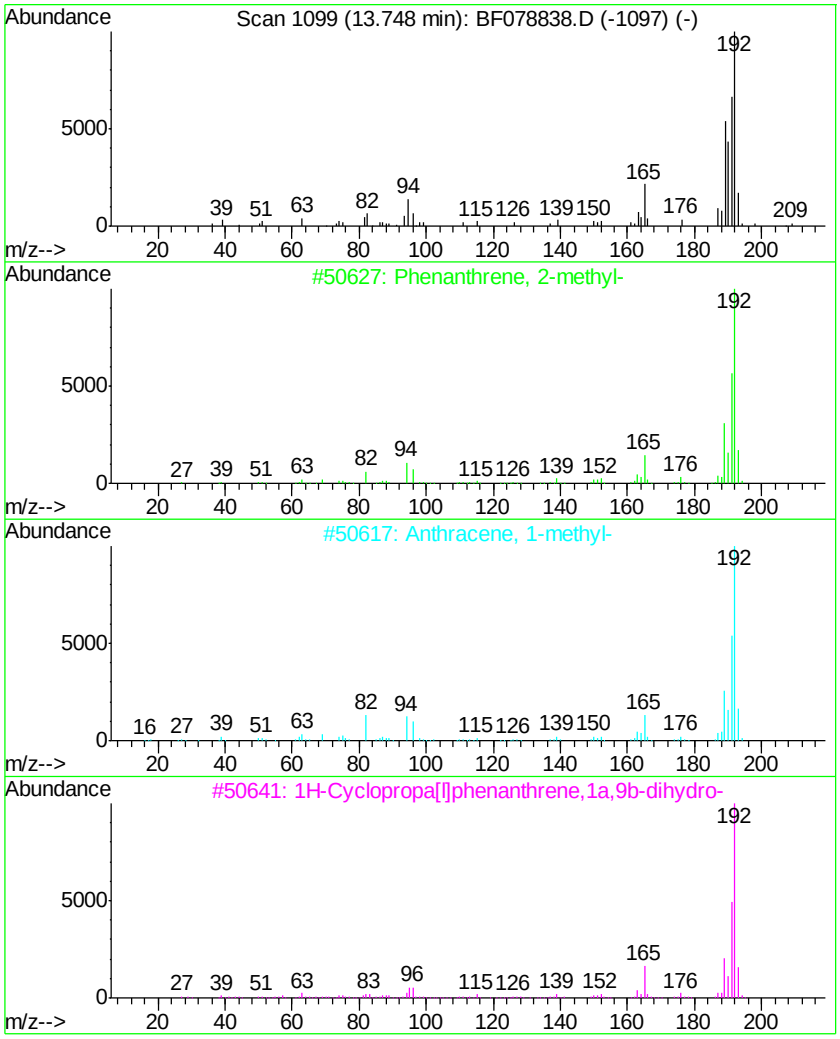
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

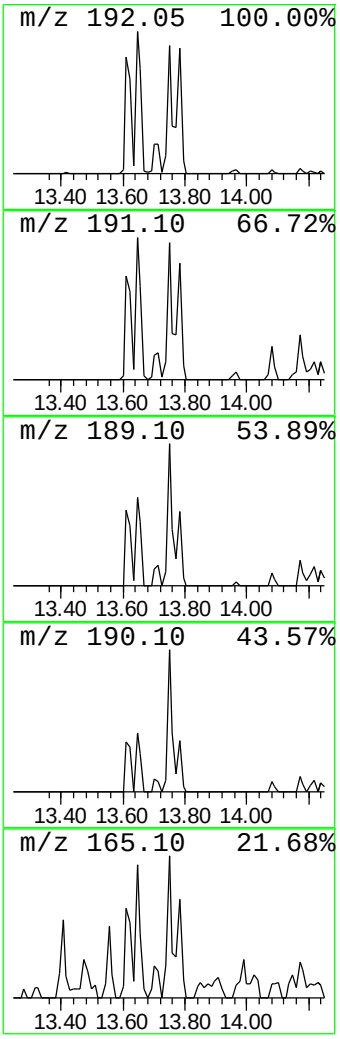
****

Peak Number 12 Anthracene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.14 ng	131657	Phenanthrene-d10	12.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	92
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	91
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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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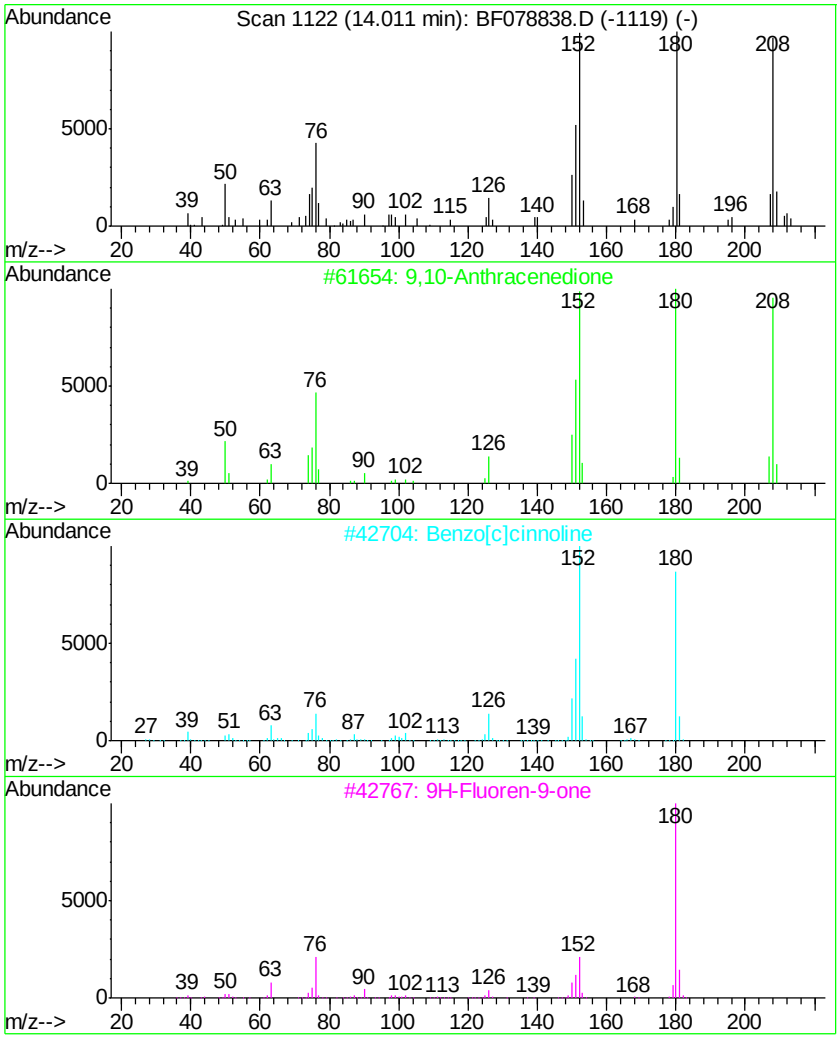
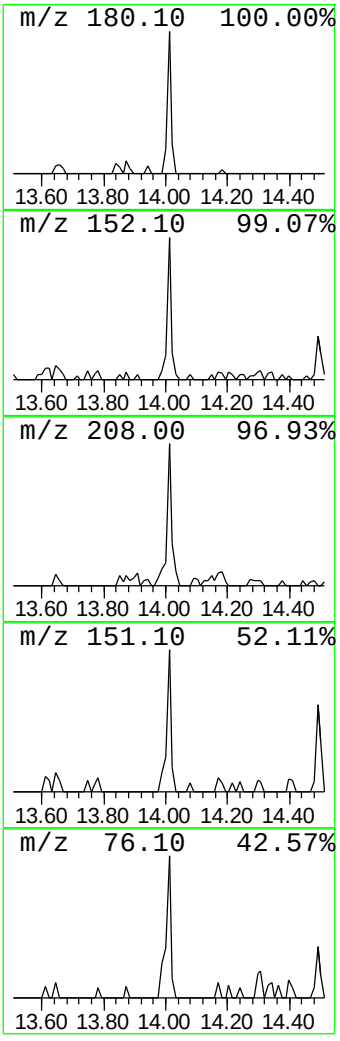
Peak Number 13 9,10-Anthracenedione Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	2.81 ng	117782	Phenanthrene-d10	12.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,10-Anthracenedione	208	C14H8O2	000084-65-1	99
2	Benzo[c]cinnoline	180	C12H8N2	000230-17-1	94
3	9H-Fluoren-9-one	180	C13H8O	000486-25-9	78
4	1H-Phenalen-1-one	180	C13H8O	000548-39-0	64
5	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	55





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

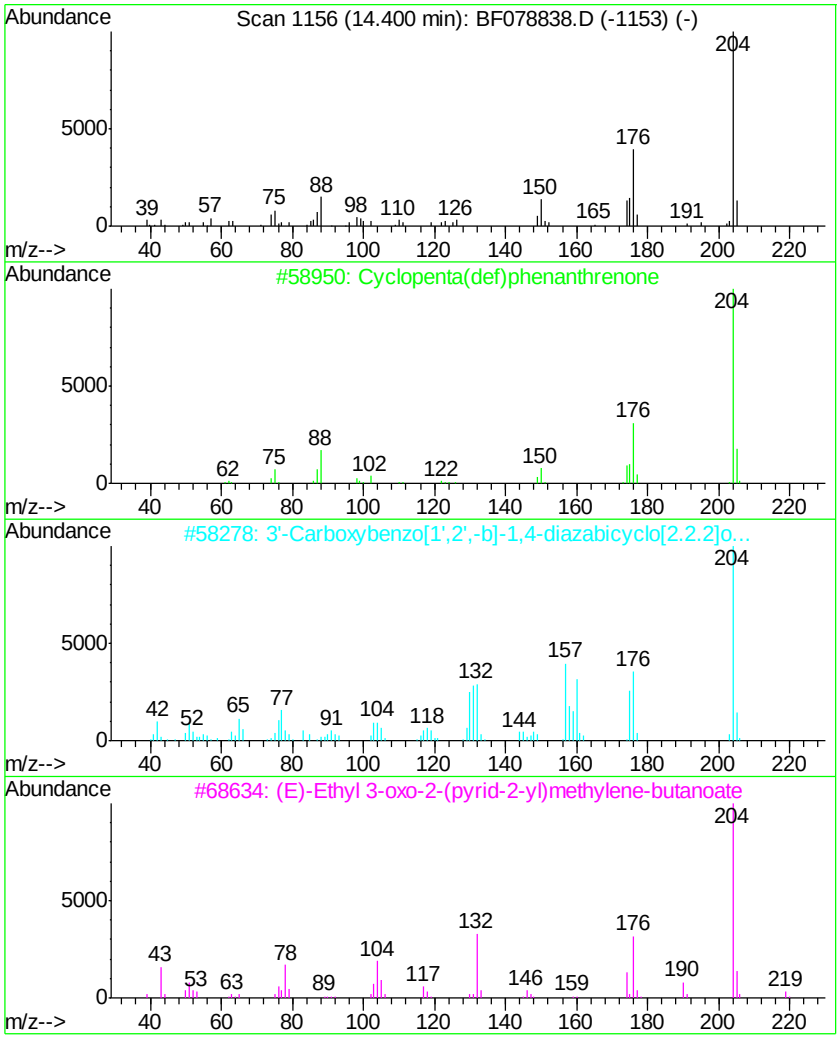
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

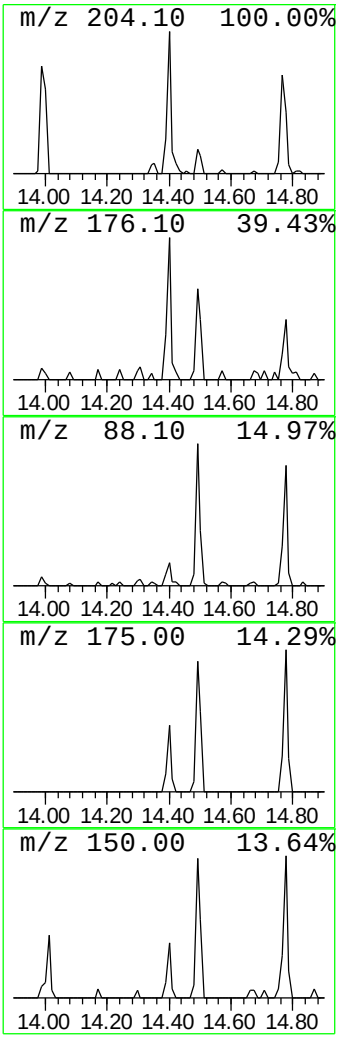
****

Peak Number 14 Cyclopenta(def)phenanthrenone Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	2.26 ng	94662	Phenanthrene-d10	12.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	90
2	3'-Carboxybenzo[1',2',-b]-1,4-di...	204	C11H12N2O2	138023-41-3	53
3	(E)-Ethyl 3-oxo-2-(pyrid-2-yl)me...	219	C12H13NO3	1000147-59-7	50
4	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	50
5	Pyrene, 4,5-dihydro-	204	C16H12	006628-98-4	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

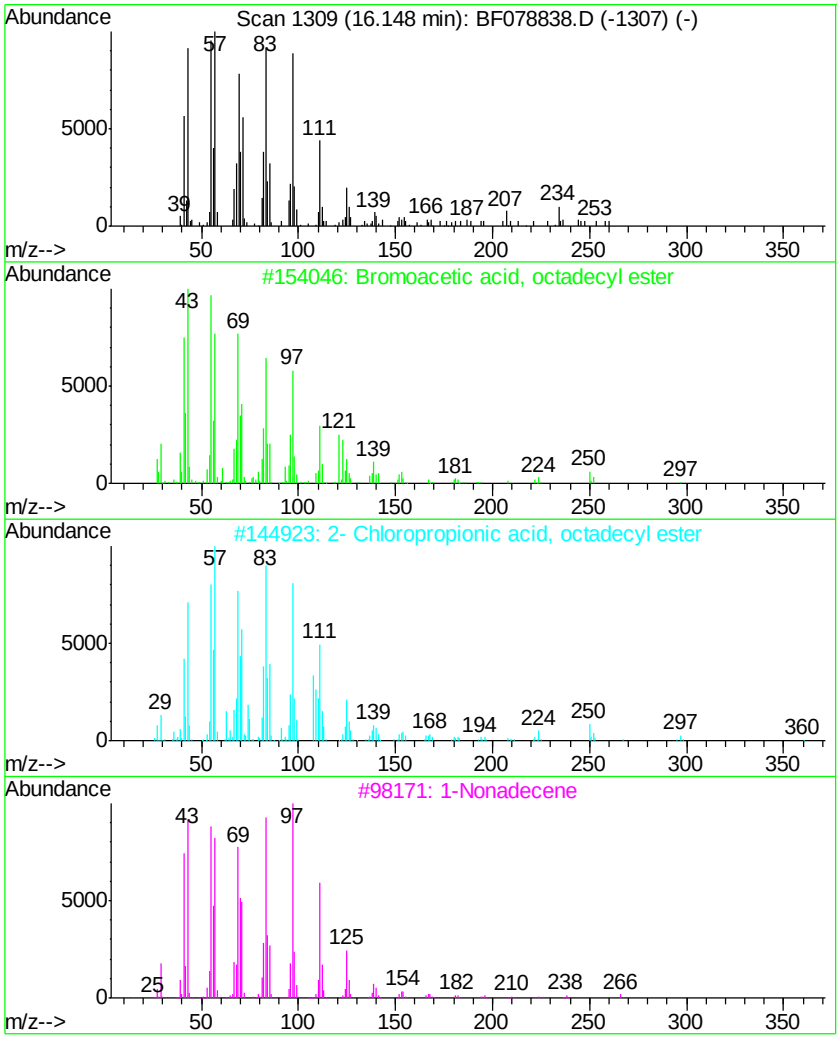
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

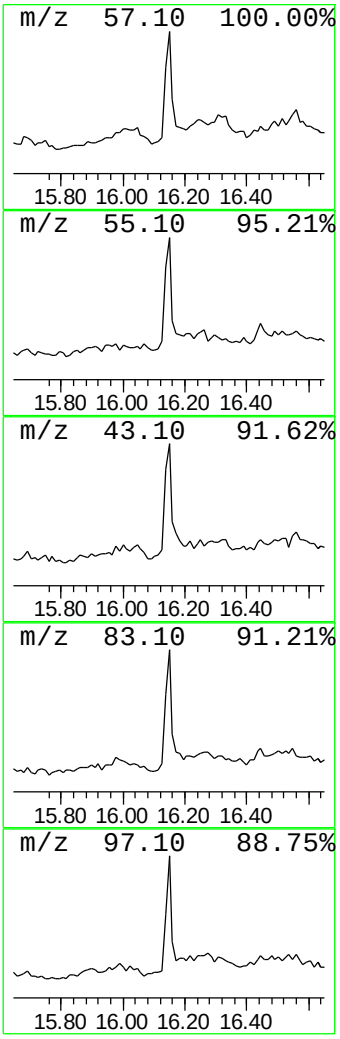
****

Peak Number 15 Bromoacetic acid, octadecyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	4.37 ng	269775	Chrysene-d12	16.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87
3	1-Nonadecene	266	C19H38	018435-45-5	86
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	83
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042915\
Data File : BF078838.D
Acq On : 30 Apr 2015 5:10
Operator : TP/IZ
Sample : G2021-07
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PS-18-2-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042815.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
unknown1.29	1.29	37.4	ng	831835	1	7.38	445484	20.0
Propane, 2,2-dime...	1.53	109.3	ng	2434570	1	7.38	445484	20.0
Butane, 2-methoxy...	1.86	12.0	ng	267664	1	7.38	445484	20.0
2-Pentanone, 4-hy...	5.19	5.1	ng	112864	1	7.38	445484	20.0
unknown7.08	7.08	36.7	ng	817887	1	7.38	445484	20.0
Anthracene, 2-met...	13.61	2.3	ng	94719	4	12.98	839219	20.0
Anthracene, 1-met...	13.75	3.1	ng	131657	4	12.98	839219	20.0
9,10-Anthracenedione	14.01	2.8	ng	117782	4	12.98	839219	20.0
Cyclopenta(def)ph...	14.40	2.3	ng	94662	4	12.98	839219	20.0
Bromoacetic acid,...	16.15	4.4	ng	269775	5	16.27	1233640	20.0