LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097500.D
Acq On : 9 Aug 2017 6:02
Operator : SJ/JU
Sample : I4604-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-080217

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-BF072517.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	4.534	464	467	483	rBV	52389	102990	4.15%	0.541%
2	5.004	544	547	570	rBV	1132355	1622624	65.42%	8.516%
3	5.645	652	656	665	rBV	24535	35652	1.44%	0.187%
4	6.081	727	730	740	rBV	763784	1027778	41.44%	5.394%
5	6.181	744	747	761	rVB	2426546	2480356	100.00%	13.018%
6	6.292	761	766	779	rVB2	64061	118954	4.80%	0.624%
7	6.404	782	785	792	rBV	636063	599985	24.19%	3.149%
8	6.463	792	795	799	rBV	32677	37052	1.49%	0.194%
9	6.563	808	812	822	rBV	2256539	2241186	90.36%	11.763%
10	6.757	843	845	850	rBV	34124	37395	1.51%	0.196%
11	6.981	879	883	900	rBV	1891610	1986056	80.07%	10.424%
12	7.686	1000	1003	1015	rBV	684801	694094	27.98%	3.643%
13	8.710	1174	1177	1182	rBV	64986	64386	2.60%	0.338%
14	8.769	1182	1187	1190	rBV	2565743	2477803	99.90%	13.005%
15	9.169	1252	1255	1263	rVB	100021	95902	3.87%	0.503%
16	9.433	1296	1300	1310	rBV	727123	647572	26.11%	3.399%
17	10.222	1430	1434	1446	rVB	1238171	1204882	48.58%	6.324%
18	10.357	1454	1457	1467	rVB	21791	27860	1.12%	0.146%
19	10.904	1547	1550	1560	rBV	597546	556945	22.45%	2.923%
20	11.139	1586	1590	1601	rBV	47148	85446	3.44%	0.448%
21	12.292	1782	1786	1792	rBV	82482	109153	4.40%	0.573%
22	12.492	1815	1820	1823	rBV	1735920	1702232	68.63%	8.934%
23	13.292	1951	1956	1962	rBV	52296	76151	3.07%	0.400%
24	13.433	1973	1980	1993	rBV4	38874	98666	3.98%	0.518%
25	13.533	1993	1997	2006	rBV	425042	455216	18.35%	2.389%
26	14.174	2103	2106	2112	rBV2	28341	36789	1.48%	0.193%
27	14.874	2220	2225	2229	rBV	309535	397463	16.02%	2.086%
28	15.251	2285	2289	2293	rVB5	20675	32158	1.30%	0.169%

Sum of corrected areas: 19052746

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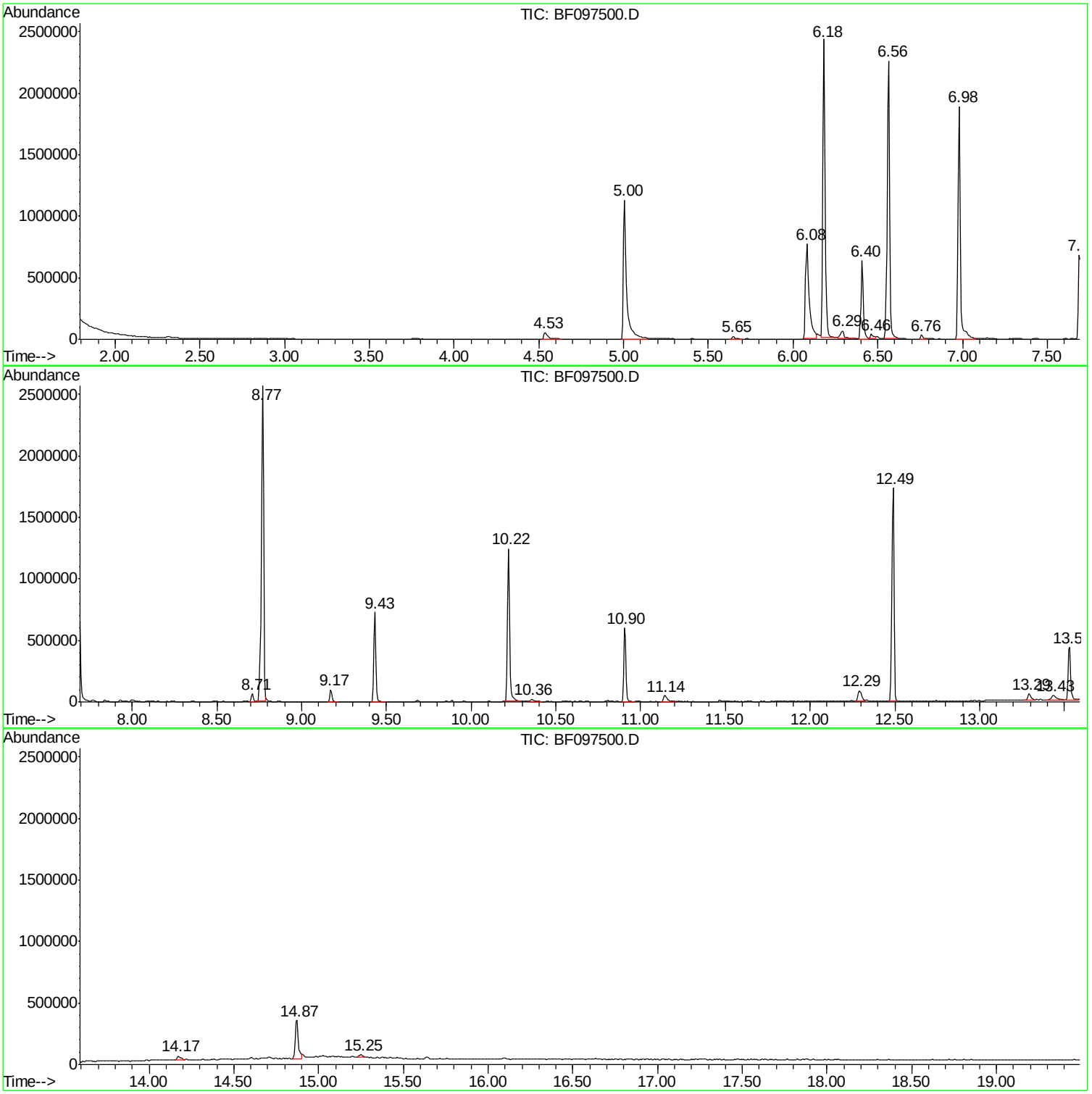
Instrument :
BNA_F
ClientSampleId :
MW-5A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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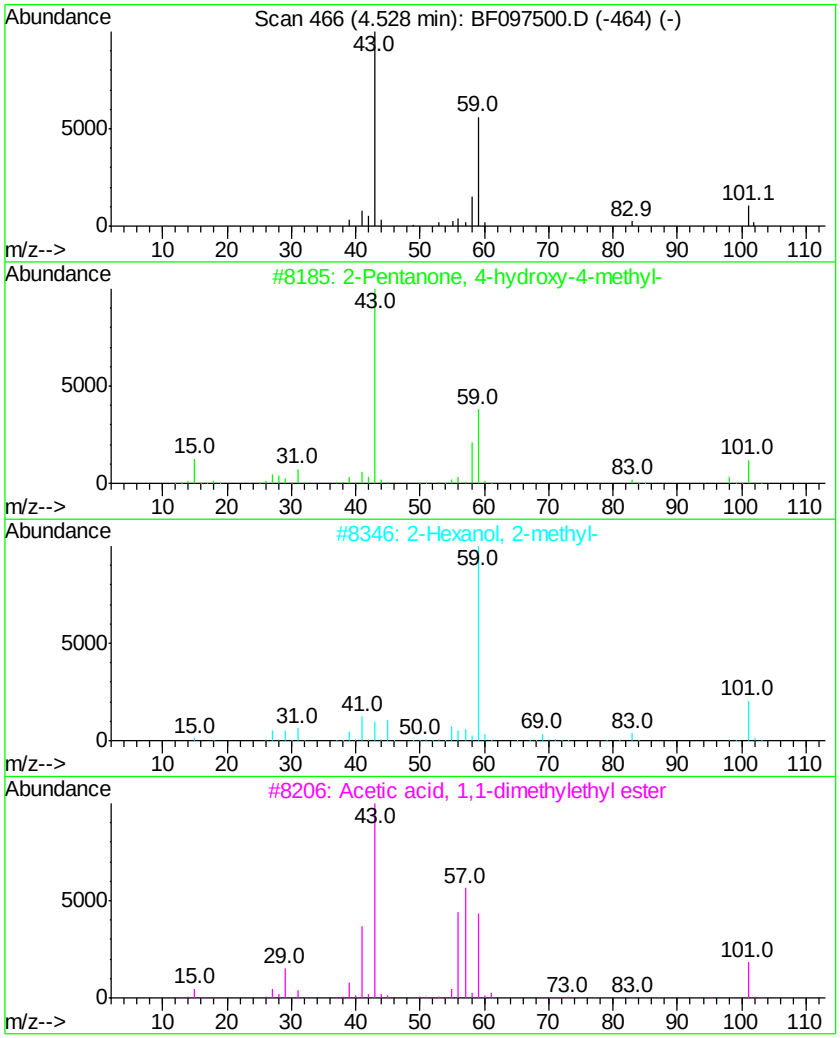
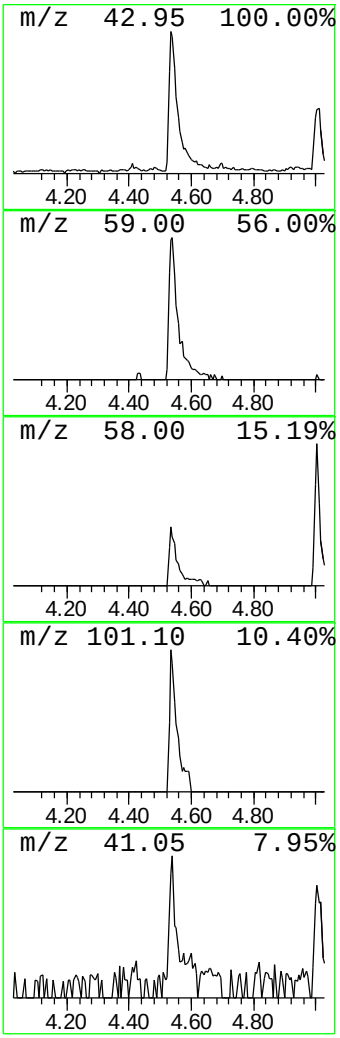
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	3.43 ng	102990	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	3-Octanol	130	C8H18O	000589-98-0	28





Library Search Compound Report

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Operator : SJ/JU
Sample : I4604-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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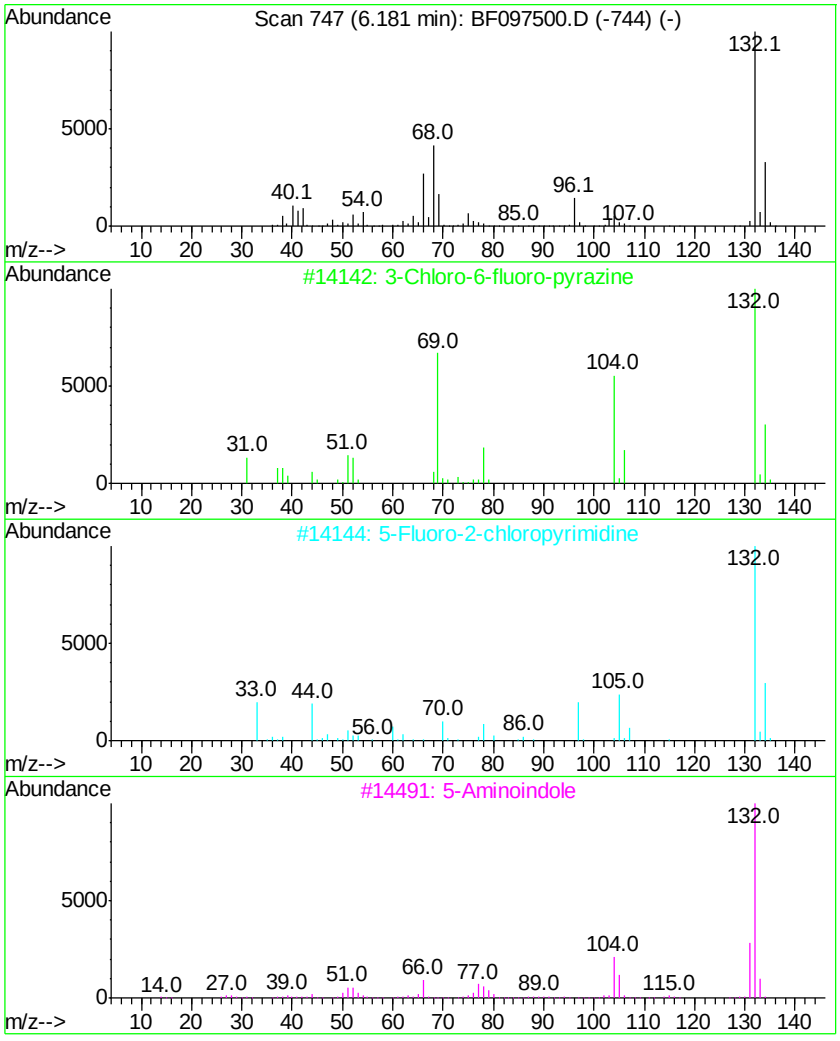
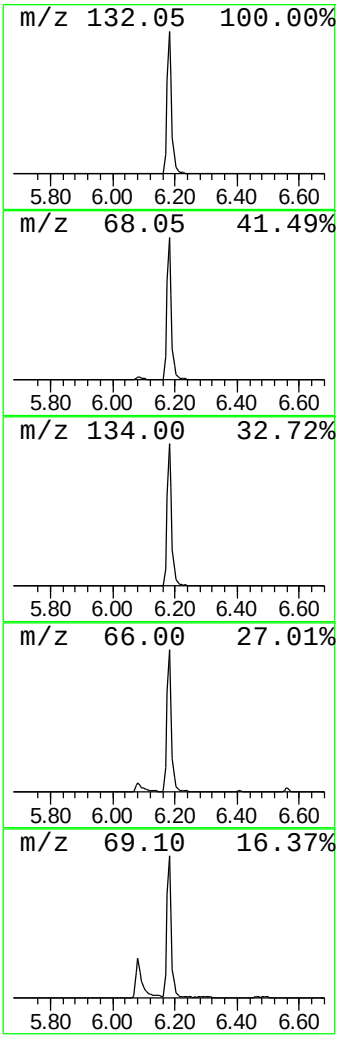
Peak Number 2 unknown6.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	82.68 ng	2480360	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
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	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
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Sample : I4604-06
Misc :
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Instrument : BNA_F
ClientSampleId : MW-5A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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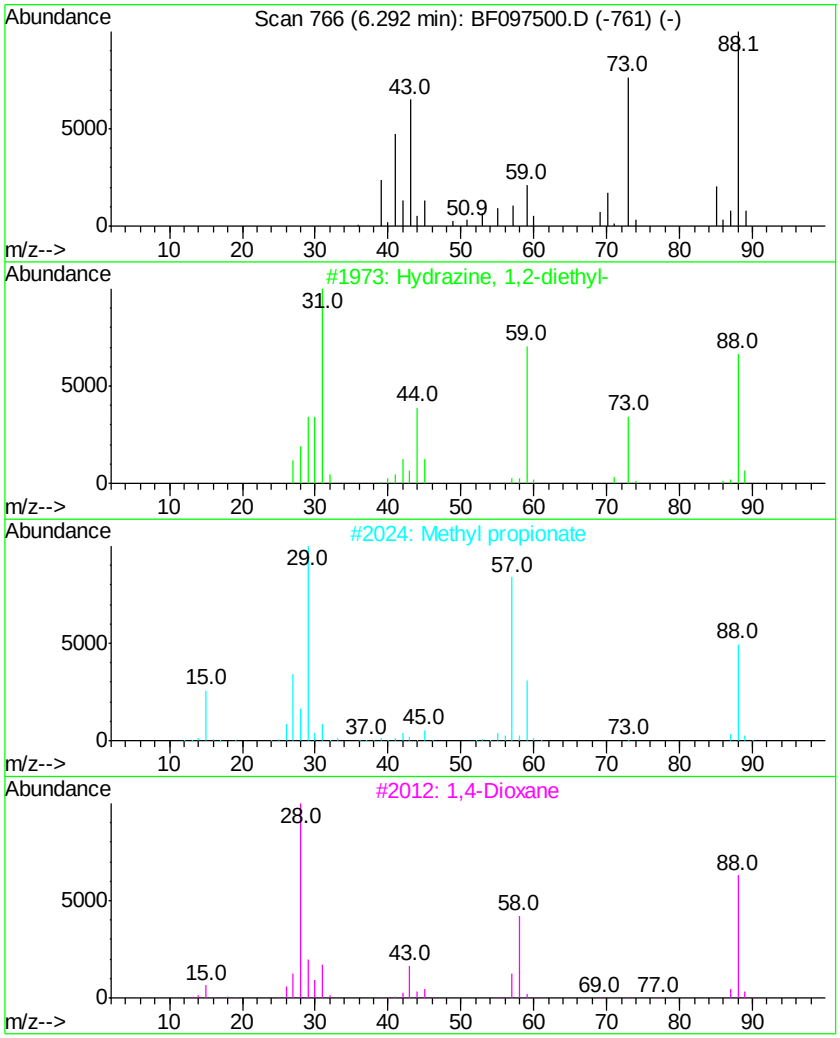
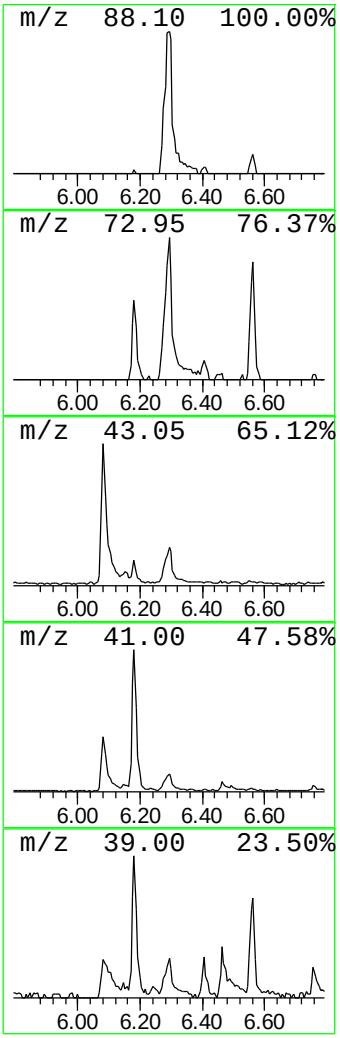
Peak Number 3 unknown6.29 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	3.97 ng	118954	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	38
2	Methyl propionate	88	C4H8O2	000554-12-1	38
3	1,4-Dioxane	88	C4H8O2	000123-91-1	32
4	dl-Aspartic acid	133	C4H7NO4	000617-45-8	23
5	Aspartic acid	133	C4H7NO4	000056-84-8	23





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Sample : I4604-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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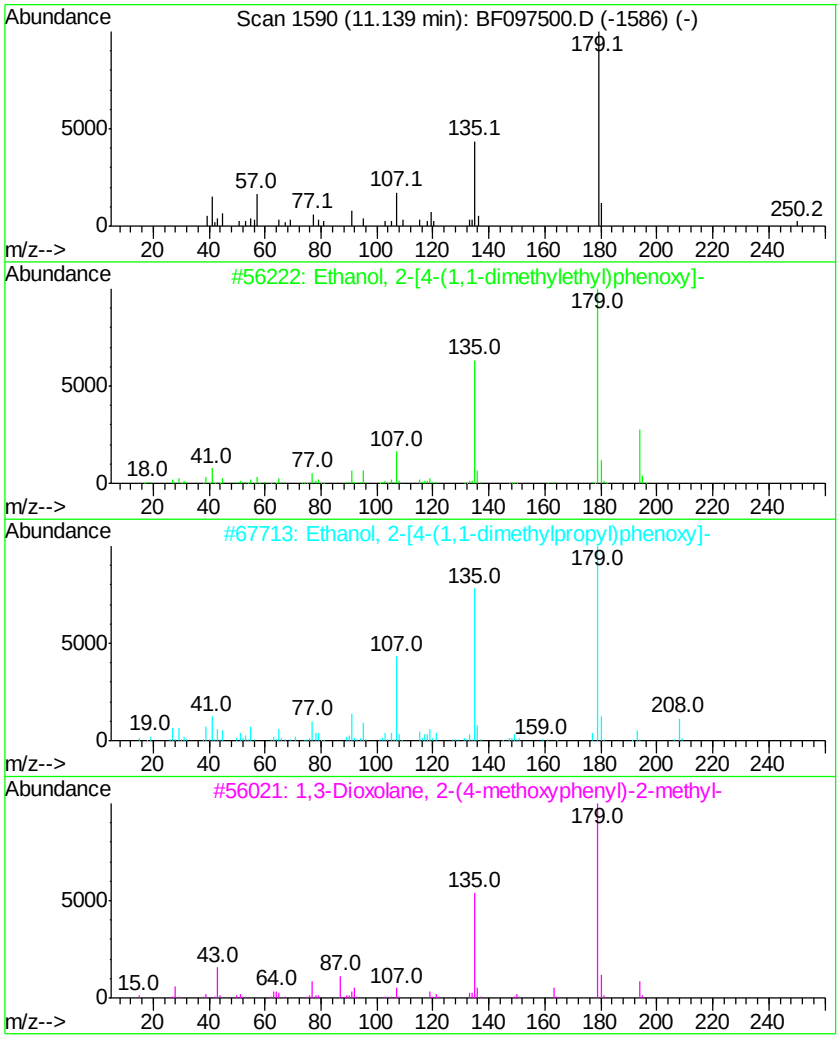
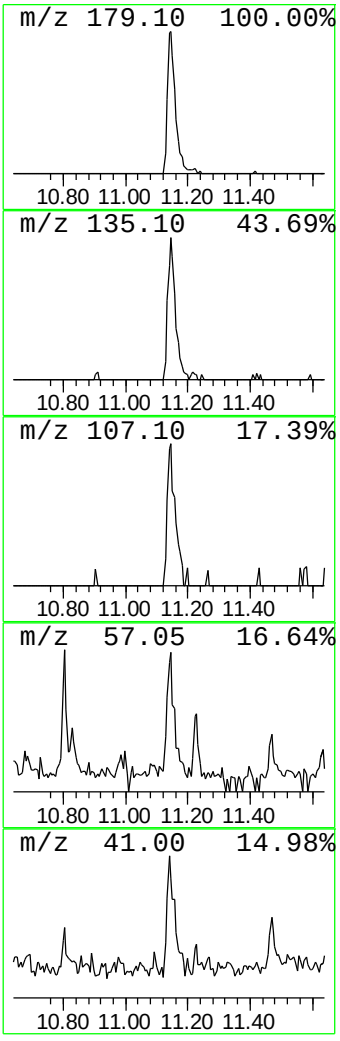
Peak Number 5 Ethanol, 2-[4-(1,1-dimethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	3.07 ng	85446	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-[4-(1,1-dimethylethyl...	194	C12H18O2	000713-46-2	64
2	Ethanol, 2-[4-(1,1-dimethylpropy...	208	C13H20O2	006382-07-6	64
3	1,3-Dioxolane, 2-(4-methoxyphenv...	194	C11H14O3	036881-00-2	50
4	2-(4-Formyl-phenoxy)-acetamide	179	C9H9NO3	135857-20-4	39
5	1-Dimethyl(phenyl)silyloxypropane	194	C11H18OSi	013360-21-9	38





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Sample : I4604-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-5A-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

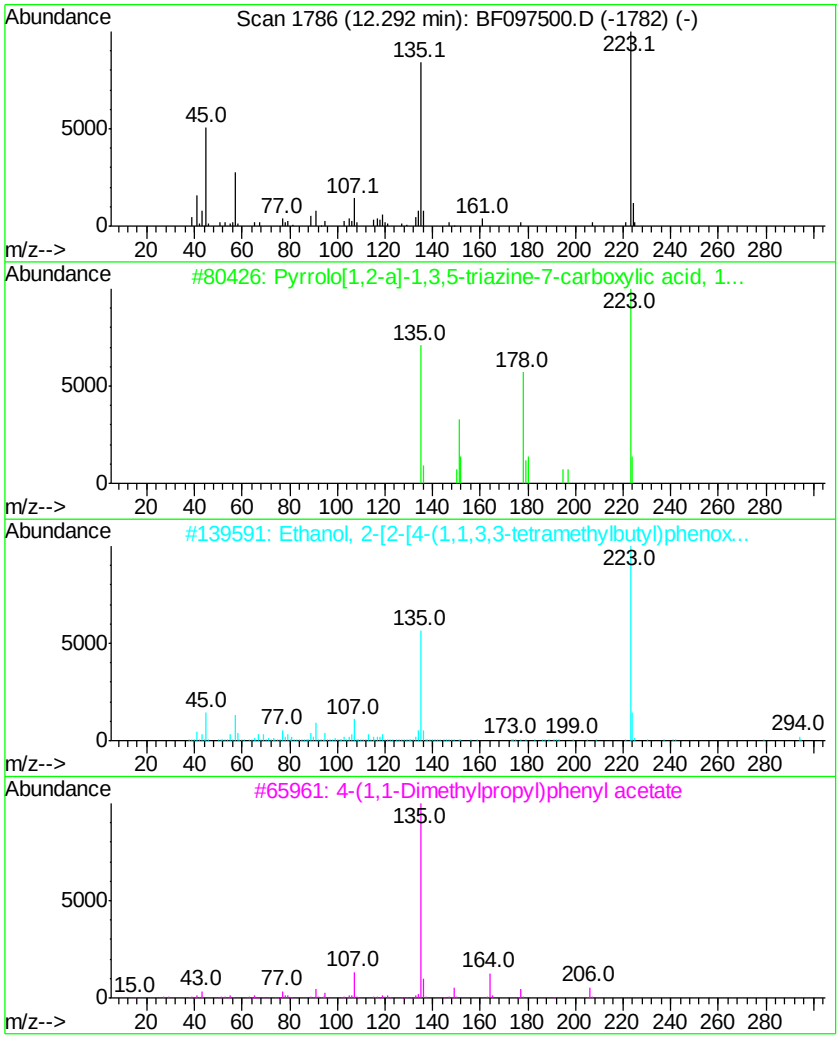
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

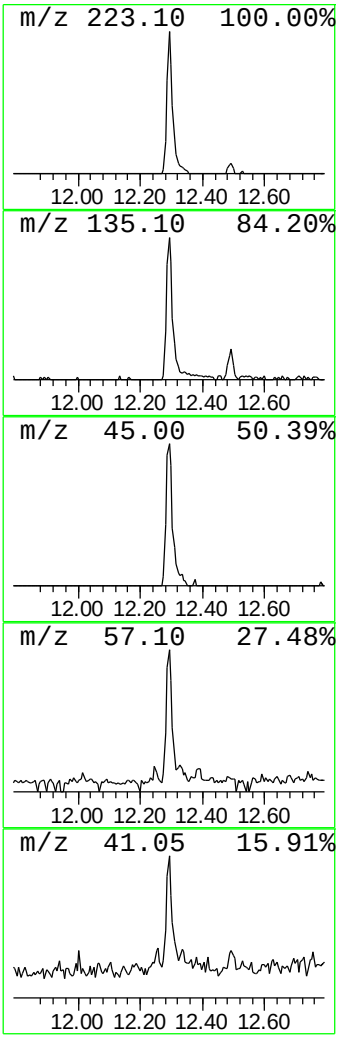
****

Peak Number 6 Pyrrolo[1,2-a]-1,3,5-triazi... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	4.80 ng	109153	Chrysene-d12	13.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrrolo[1,2-a]-1,3,5-triazine-7-...	223	C9H9N3O4	054449-89-7	90
2	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	52
3	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	27
4	o-Anisic acid, 2,6-dimethylnon-1...	300	C19H24O3	1000292-57-7	22
5	2-Methyl-2-(4'-hydroxyphenyl)pen...	192	C12H16O2	070205-18-4	16





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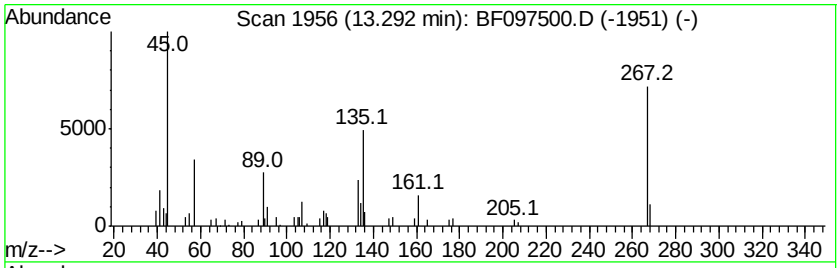
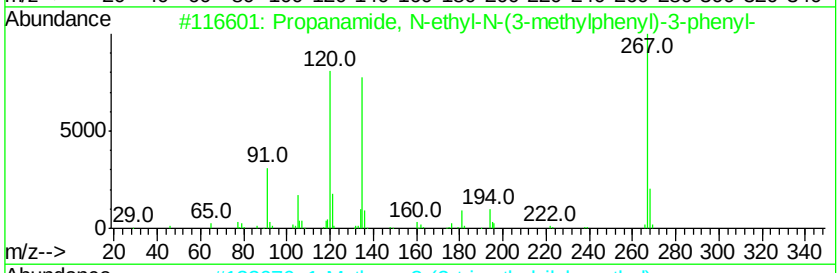
****

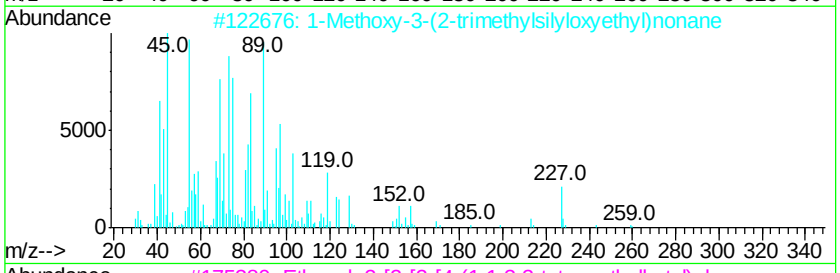
Peak Number 7 unknown13.29 Concentration Rank 7

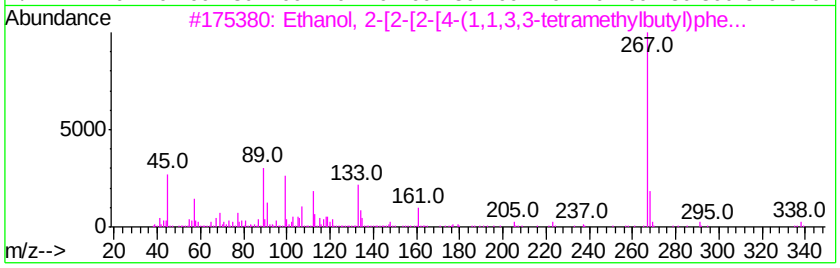
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	3.35 ng	76151	Chrysene-d12	13.53

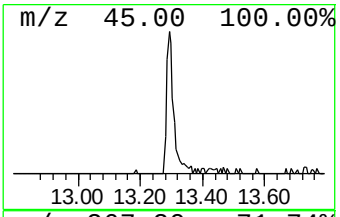
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanamide, N-ethyl-N-(3-methyl...	267	C18H21NO	1000308-21-3	38
2	1-Methoxy-3-(2-trimethylsilyloxy...	274	C15H34O2Si	1000216-82-7	16
3	Ethanol, 2-[2-[2-[4-(1,1,3,3-tet...	338	C20H34O4	002315-62-0	16
4	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	12
5	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	12

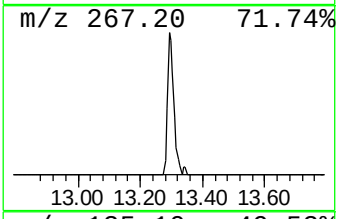


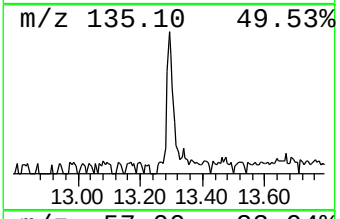


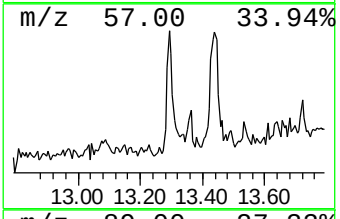


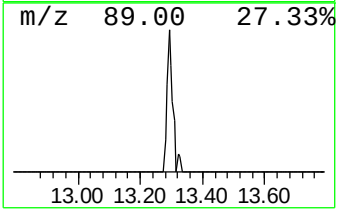












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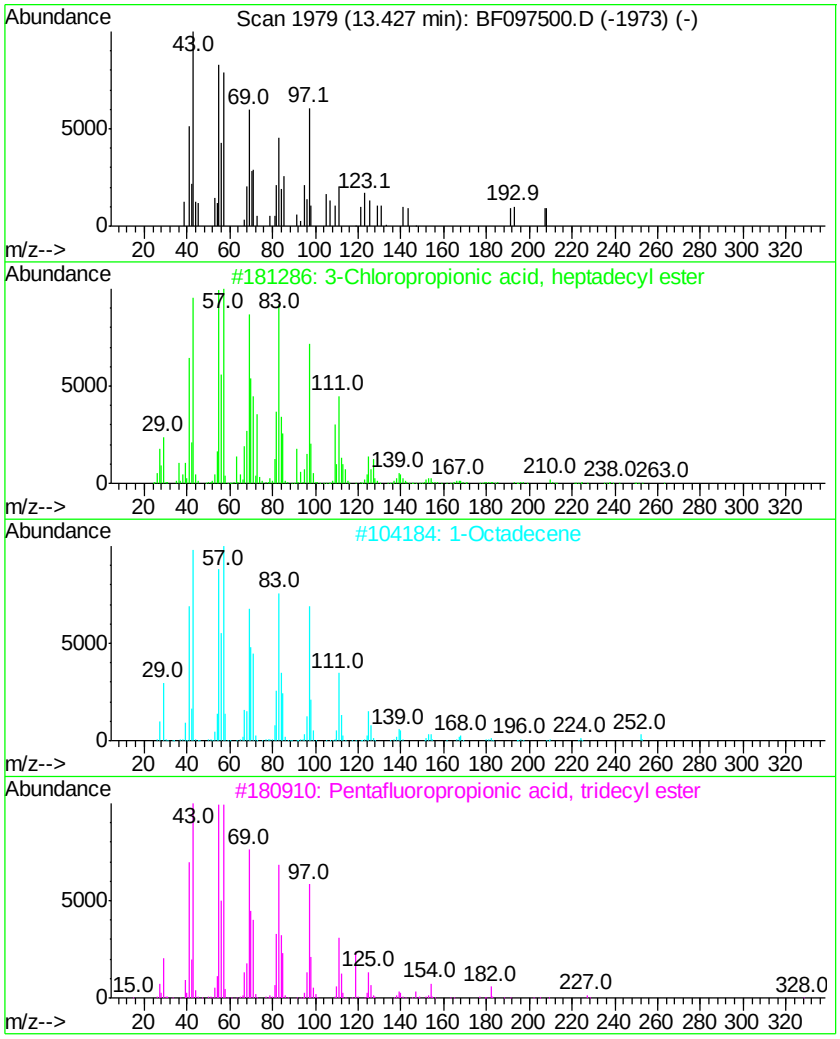
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

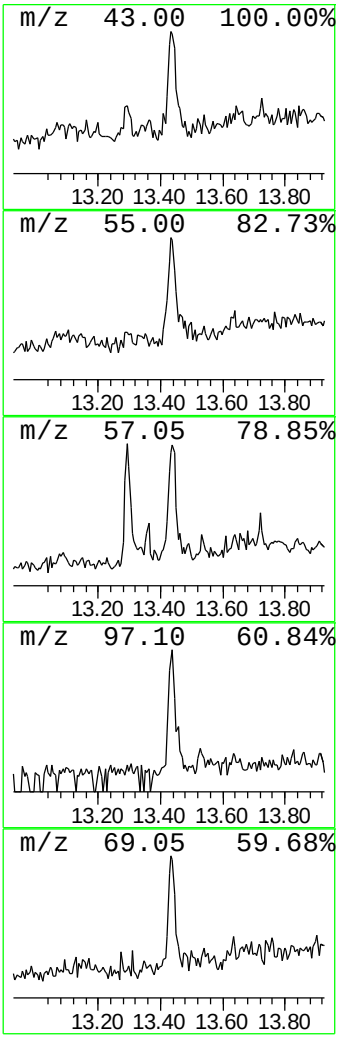
****

Peak Number 8 3-Chloropropionic acid, hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	4.33 ng	98666	Chrysene-d12	13.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2	1-Octadecene	252	C18H36	000112-88-9	87
3	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	87
4	1-Docosene	308	C22H44	001599-67-3	87
5	11-Tricosene	322	C23H46	052078-56-5	83





Tentatively Identified Compound (LSC) summary

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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...	4.53	3.4	ng	102990	1	6.40	599985	20.0
unknown6.18	6.18	82.7	ng	2480360	1	6.40	599985	20.0
unknown6.29	6.29	4.0	ng	118954	1	6.40	599985	20.0
Ethanol, 2-[4-(1,...	11.14	3.1	ng	85446	4	10.90	556945	20.0
Pyrrolo[1,2-a]-1,...	12.29	4.8	ng	109153	5	13.53	455216	20.0
unknown13.29	13.29	3.4	ng	76151	5	13.53	455216	20.0
3-Chloropropionic...	13.43	4.3	ng	98666	5	13.53	455216	20.0