LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097492.D
Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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	4.540	464	468	482	rBV	120383	220384	9.67%	1.157%
2	5.004	543	547	573	rBV	1842367	2279242	100.00%	11.971%
3	6.081	726	730	743	rBV	1994793	2188258	96.01%	11.493%
4	6.181	743	747	757	rVB	2169946	2150670	94.36%	11.296%
5	6.404	782	785	798	rBV	744026	684343	30.03%	3.594%
6	6.563	808	812	825	rBV	1318287	1300312	57.05%	6.829%
7	6.981	879	883	895	rBV	1230333	1258079	55.20%	6.608%
8	7.686	1000	1003	1013	rBV	844314	824768	36.19%	4.332%
9	8.769	1183	1187	1190	rBV	1763274	1568258	68.81%	8.237%
10	9.169	1252	1255	1262	rBV	390597	321365	14.10%	1.688%
11	9.433	1296	1300	1304	rBV	796287	732724	32.15%	3.848%
12	9.886	1374	1377	1381	rVB	28442	24657	1.08%	0.130%
13	10.222	1431	1434	1445	rBV	992459	906305	39.76%	4.760%
14	10.357	1454	1457	1464	rVB	44325	50658	2.22%	0.266%
15	10.804	1530	1533	1536	rBV3	33902	28148	1.23%	0.148%
16	10.904	1547	1550	1553	rBV	695241	664150	29.14%	3.488%
17	10.927	1553	1554	1560	rVB	55463	49239	2.16%	0.259%
18	11.469	1643	1646	1652	rBV	102252	97391	4.27%	0.512%
19	12.110	1752	1755	1761	rBV	92236	102086	4.48%	0.536%
20	12.245	1775	1778	1784	rBV2	56151	77731	3.41%	0.408%
21	12.339	1789	1794	1800	rVV	119649	136705	6.00%	0.718%
22	12.486	1815	1819	1823	rBV	1205036	1215405	53.32%	6.383%
23	12.774	1865	1868	1877	rVB6	18937	33636	1.48%	0.177%
24	13.045	1910	1914	1915	rBV4	19417	24836	1.09%	0.130%
25	13.204	1937	1941	1943	rBV5	21305	35222	1.55%	0.185%
26	13.433	1976	1980	1984	rBV2	44748	79528	3.49%	0.418%
27	13.533	1992	1997	2000	rBV	666974	708625	31.09%	3.722%
28	13.627	2008	2013	2021	rBV	31605	78812	3.46%	0.414%
29	13.762	2033	2036	2037	rBV2	24688	25935	1.14%	0.136%
30	14.180	2104	2107	2109	rBV3	40812	46548	2.04%	0.244%
31	14.210	2111	2112	2114	rVV2	36639	22867	1.00%	0.120%
32	14.245	2117	2118	2121	rBV3	33297	32917	1.44%	0.173%
33	14.298	2125	2127	2128	rBV2	32282	30428	1.34%	0.160%
34	14.380	2138	2141	2147	rBV7	38341	84536	3.71%	0.444%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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

35	14.457	2152	2154	2158	rBV5	37854	52694	2.31%	0.277%
36	14.874	2221	2225	2230	rVB	407961	435177	19.09%	2.286%
37	14.945	2233	2237	2242	rBV8	40670	116954	5.13%	0.614%
38	15.633	2352	2354	2359	rBV5	40395	57797	2.54%	0.304%
39	16.027	2419	2421	2422	rBV2	38447	35766	1.57%	0.188%
40	16.839	2557	2559	2564	rBV6	28987	52835	2.32%	0.277%
41	17.456	2662	2664	2665	rBV2	33327	28183	1.24%	0.148%
42	18.003	2755	2757	2761	rVB4	28466	35062	1.54%	0.184%
43	18.074	2767	2769	2773	rVB5	26457	33958	1.49%	0.178%
44	18.221	2790	2794	2799	rBV8	36181	106864	4.69%	0.561%

Sum of corrected areas: 19040058

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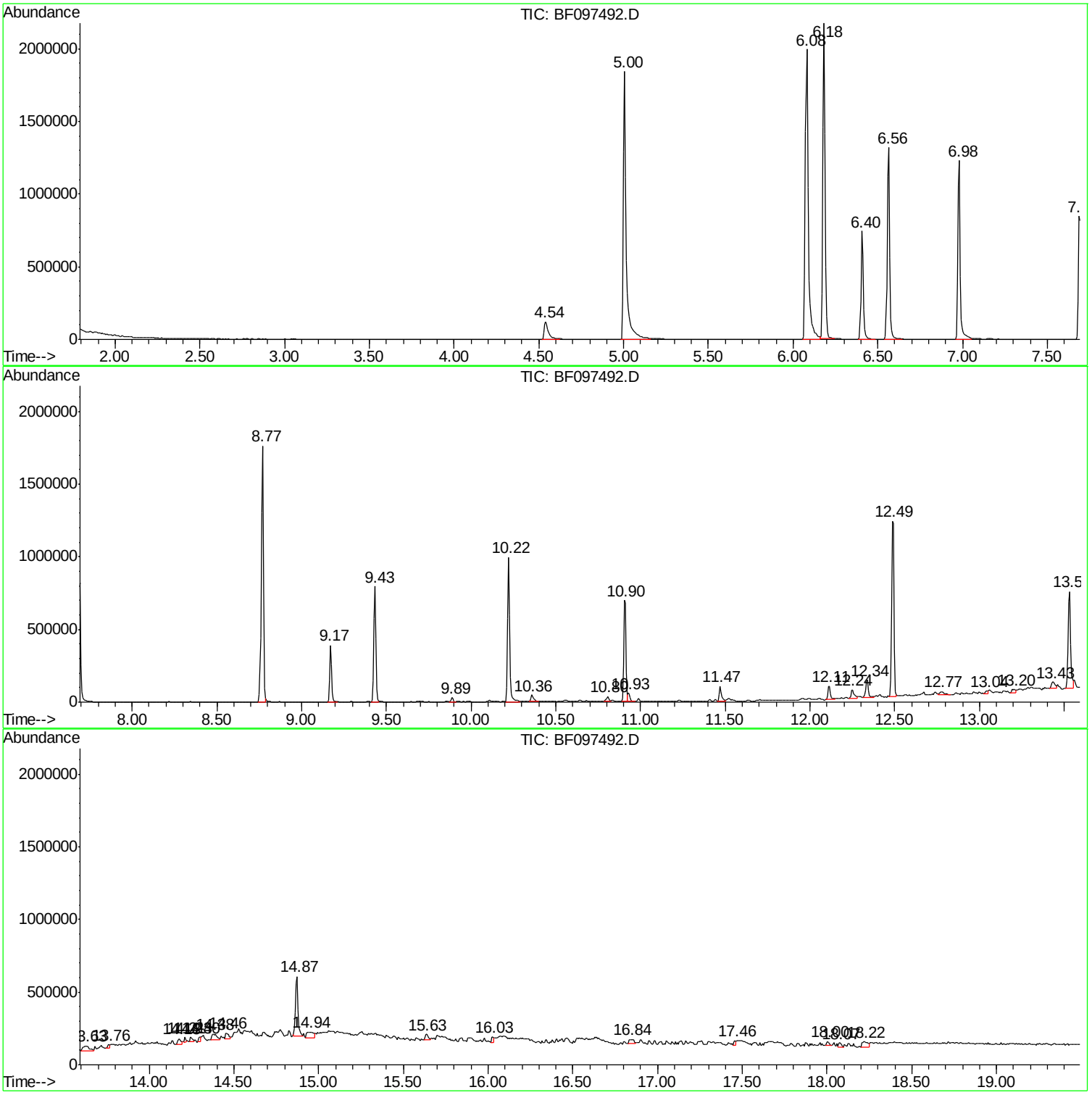
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-01-080717-B

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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Data File : BF097492.D
Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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

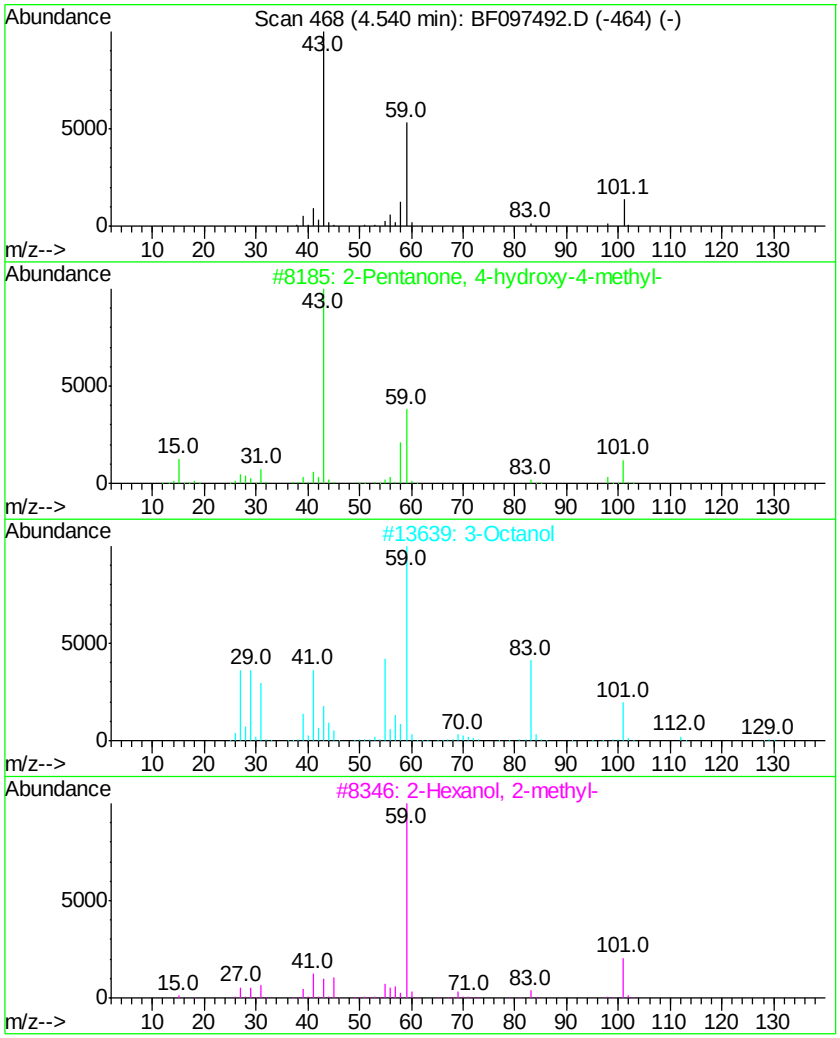
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

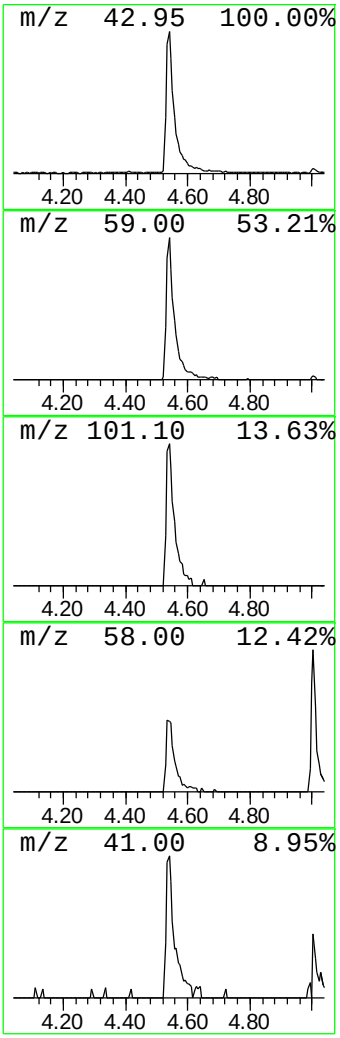
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	6.44 ng	220384	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	64
2	3-Octanol	130	C8H18O	000589-98-0	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
Data File : BF097492.D
Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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

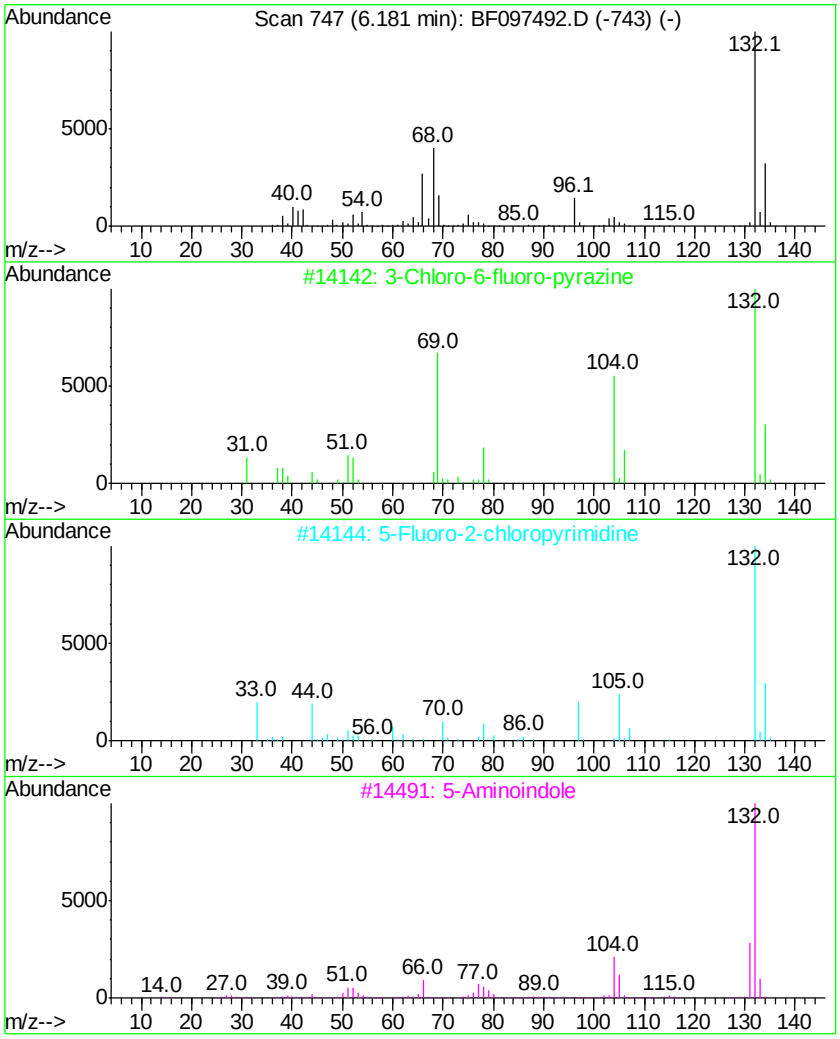
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

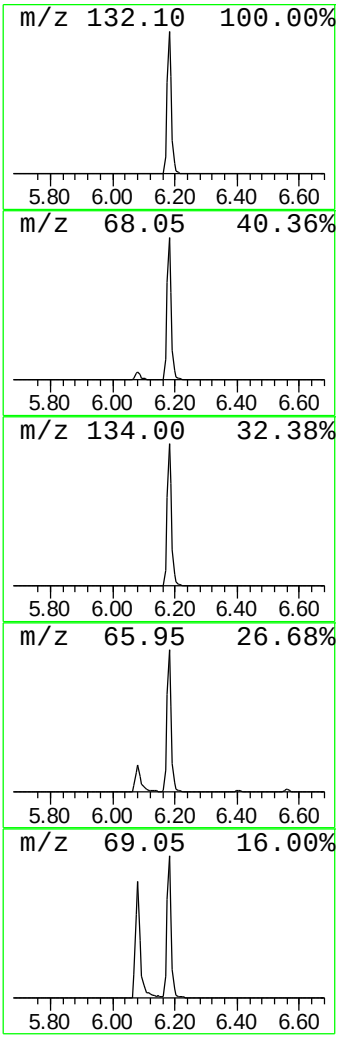
****

Peak Number 2 unknown6.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	62.85 ng	2150670	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	27
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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
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Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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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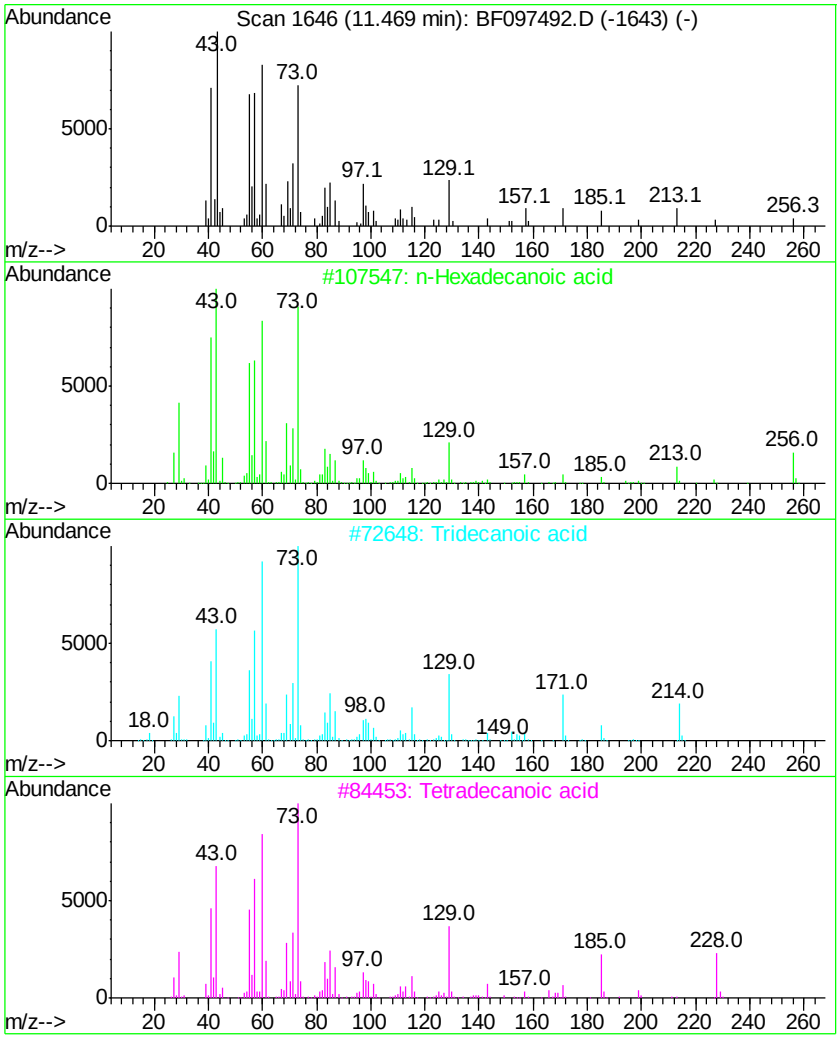
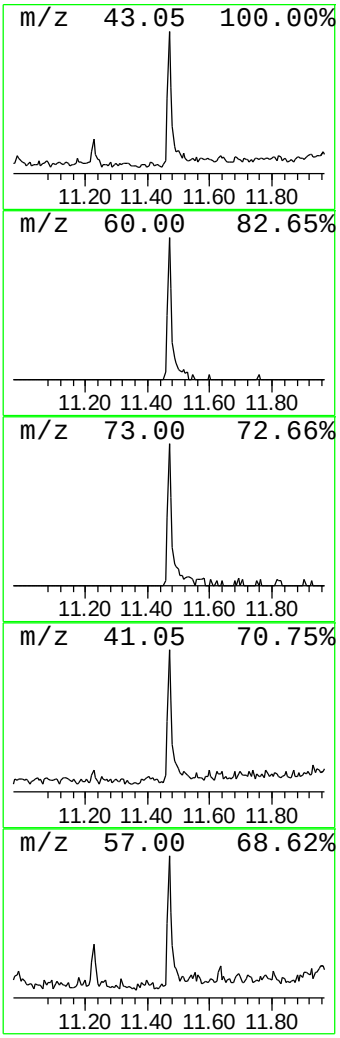
Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	2.93 ng	97391	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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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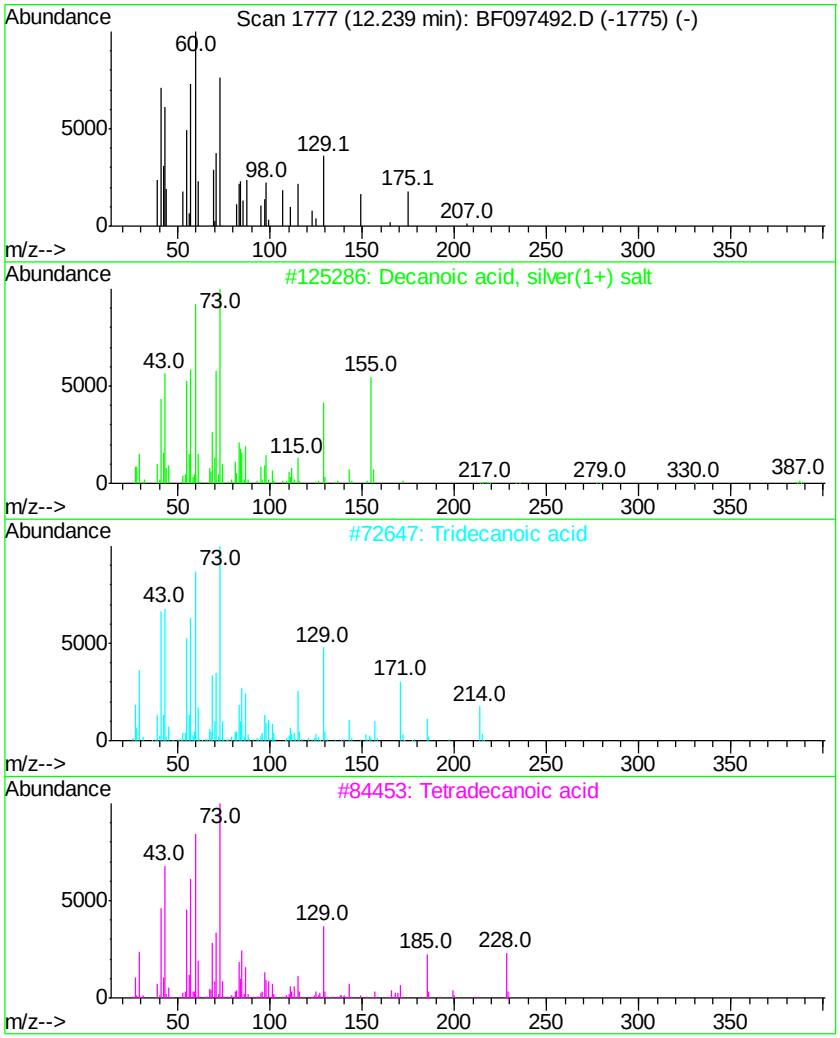
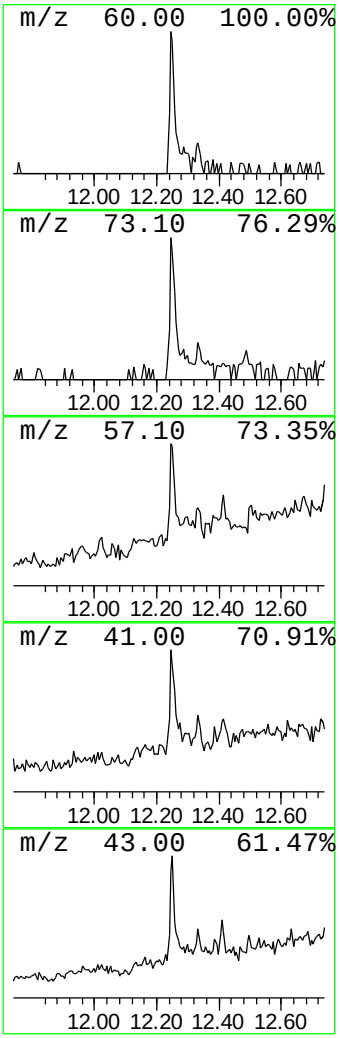
Peak Number 5 Decanoic acid, silver(1+) salt Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.24	2.19 ng	77731	Chrysene-d12	13.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59





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ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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

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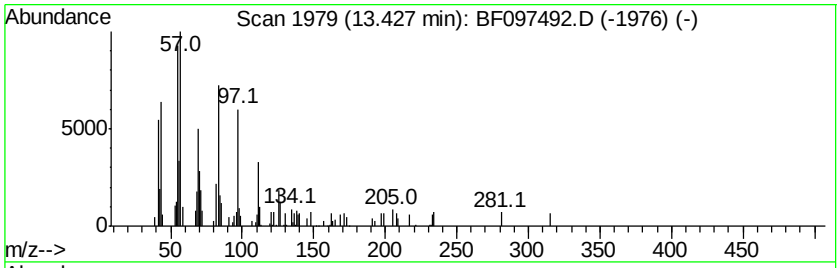
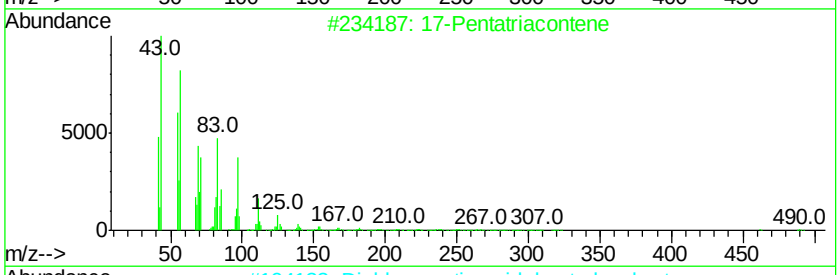
****

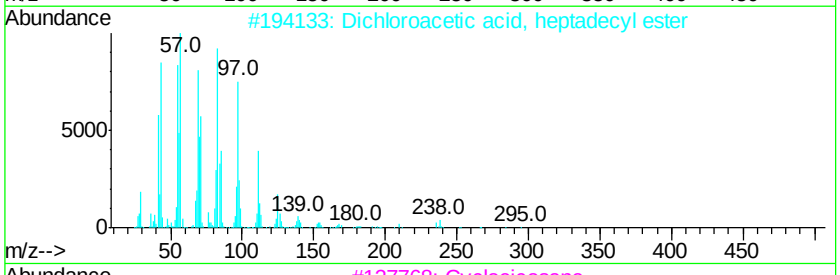
Peak Number 6 17-Pentatriacontene Concentration Rank 11

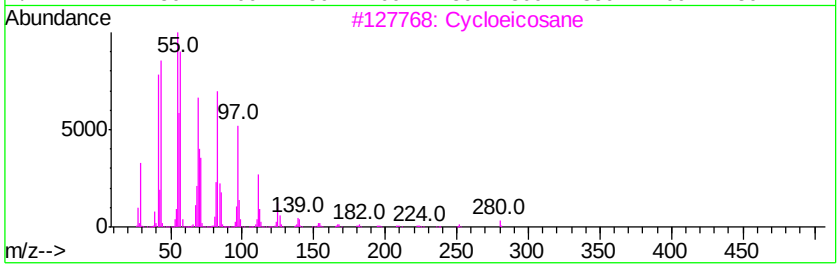
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	2.24 ng	79528	Chrysene-d12	13.53

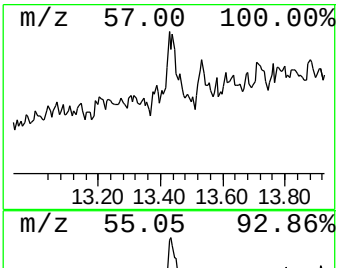
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	81
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	72
3	Cycloeicosane	280	C20H40	000296-56-0	58
4	Cyclotetradecane	196	C14H28	000295-17-0	52
5	Cyclopentadecane	210	C15H30	000295-48-7	52

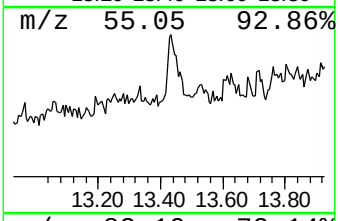


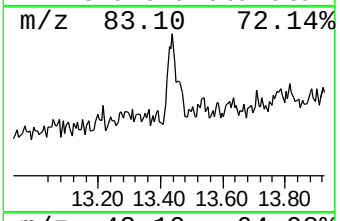


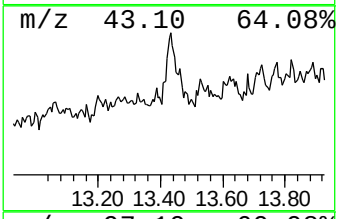


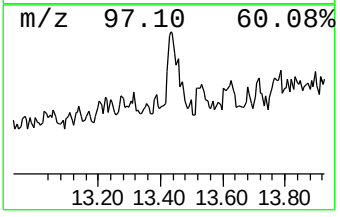












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

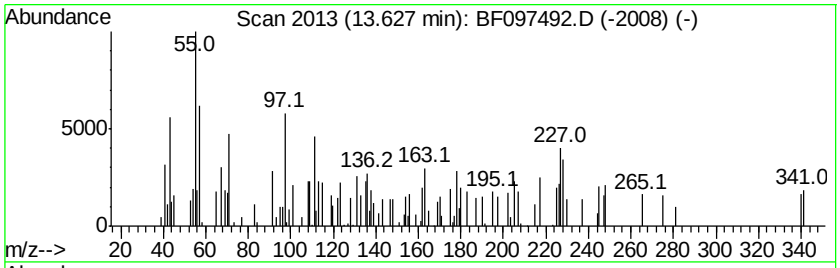
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

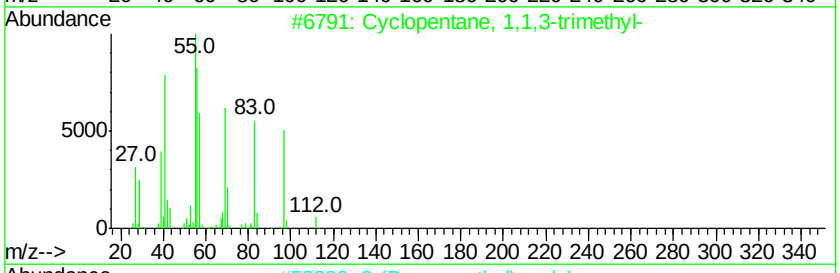
****

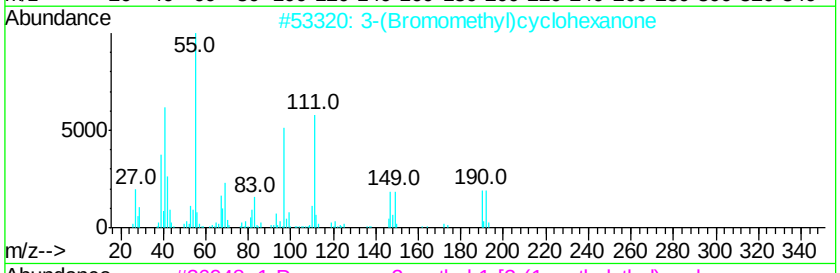
Peak Number 7 unknown13.63 Concentration Rank 12

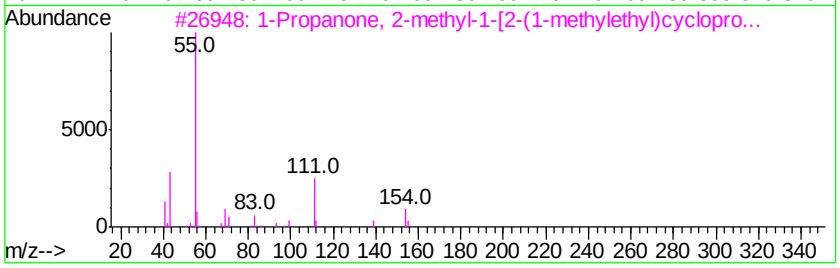
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.22 ng	78812	Chrysene-d12	13.53

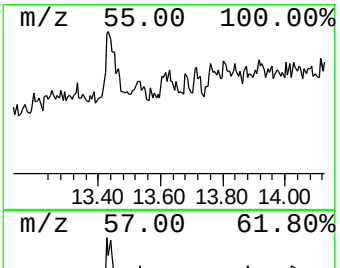
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	11
2	3-(Bromomethyl)cyclohexanone	190	C7H11BrO	168278-83-9	11
3	1-Propanone, 2-methyl-1-[2-(1-me...	154	C10H18O	056259-15-5	11
4	Tetrahydrocarvone	154	C10H18O	000499-70-7	11
5	2-Thiophenepropanoic acid, methy...	170	C8H10O2S	016862-05-8	10

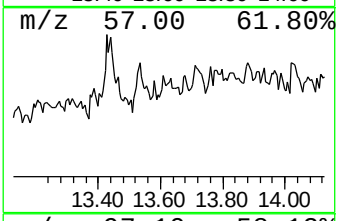


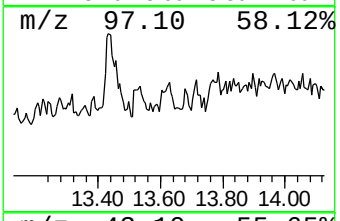


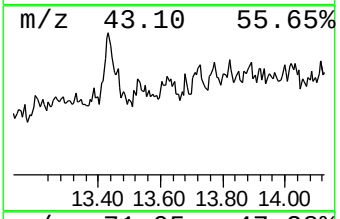


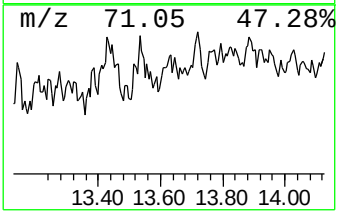












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Data File : BF097492.D
Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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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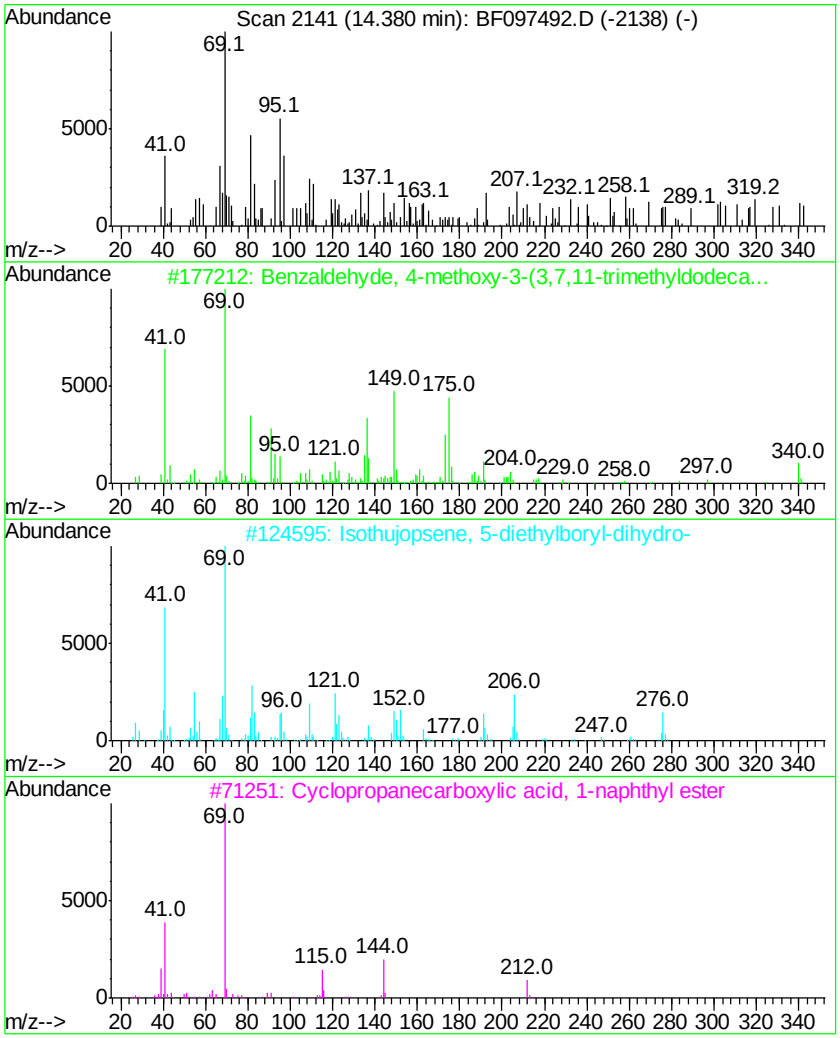
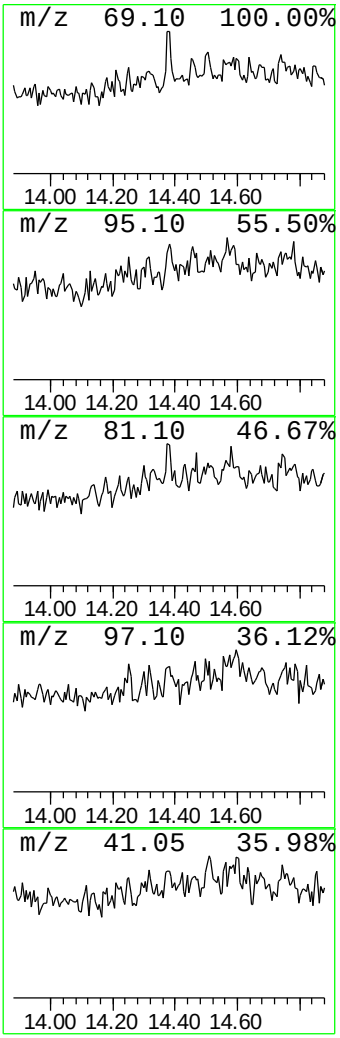
Peak Number 8 unknown14.38 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	3.89 ng	84536	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 4-methoxy-3-(3,7,1...	340	C23H32O2	1000196-52-1	35
2	Isothujopsene, 5-diethylboryl-di...	276	C19H37B	1000151-29-3	35
3	Cyclopropanecarboxylic acid, 1-n...	212	C14H12O2	1000279-96-1	30
4	6,9-Dimethyl-3-nitro-6,7-dihydro...	236	C11H12N2O4	1000210-11-6	27
5	3-Hydroxyphenol bis(trifluoroace...	302	C10H4F6O4	034065-72-0	27





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Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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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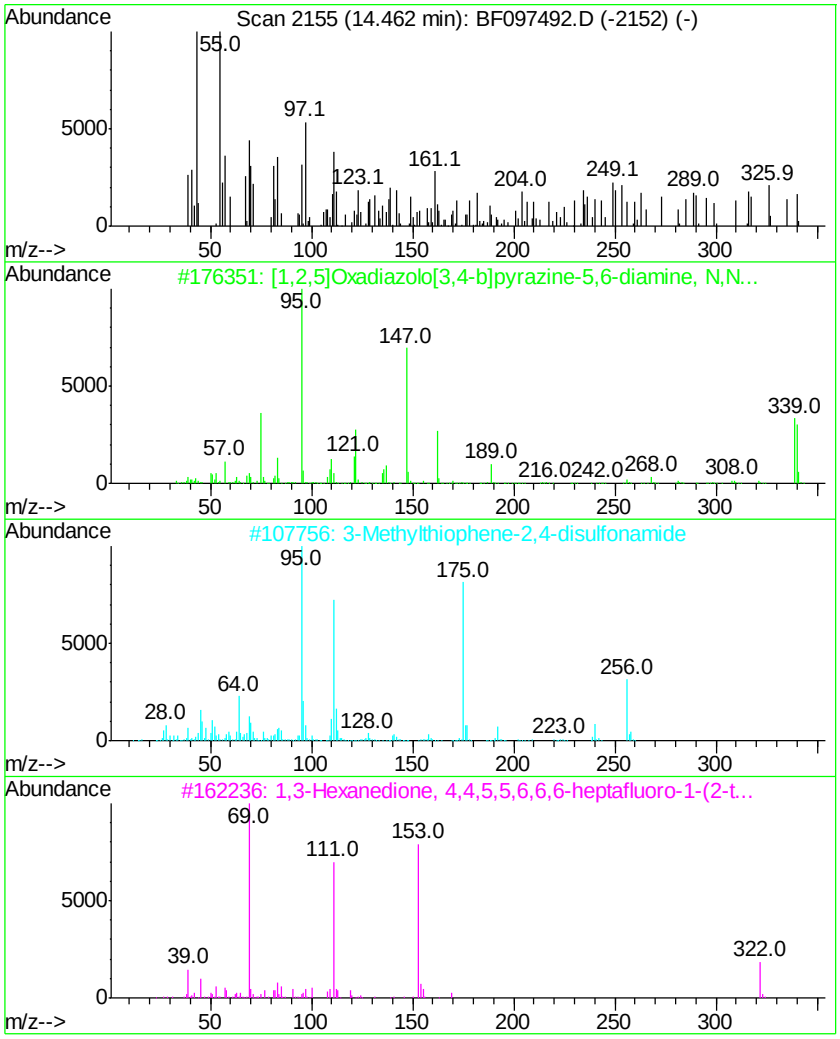
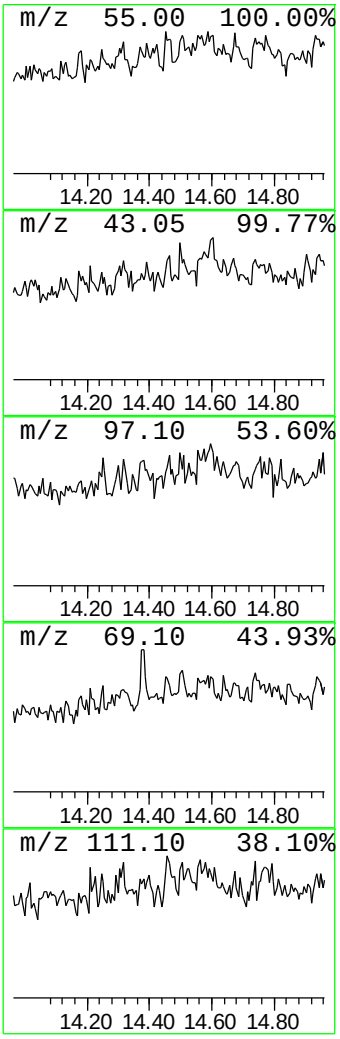
Peak Number 9 unknown14.46 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.42 ng	52694	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,2,5]Oxadiazolo[3,4-b]pyrazine...	340	C16H10F2N6O	1000316-91-4	35
2	3-Methylthiophene-2,4-disulfonamide	256	C5H8N2O4S3	104096-86-8	14
3	1,3-Hexanedione, 4,4,5,5,6,6,6-h...	322	C10H5F7O2S	000559-94-4	10
4	Furan-2-carboxamide, N-(2,4-dime...	247	C13H13NO4	328258-35-1	10
5	1H-Pyrazole-1-acetic acid, 3-[(2...	263	C12H13N3O4	1000350-47-9	10





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Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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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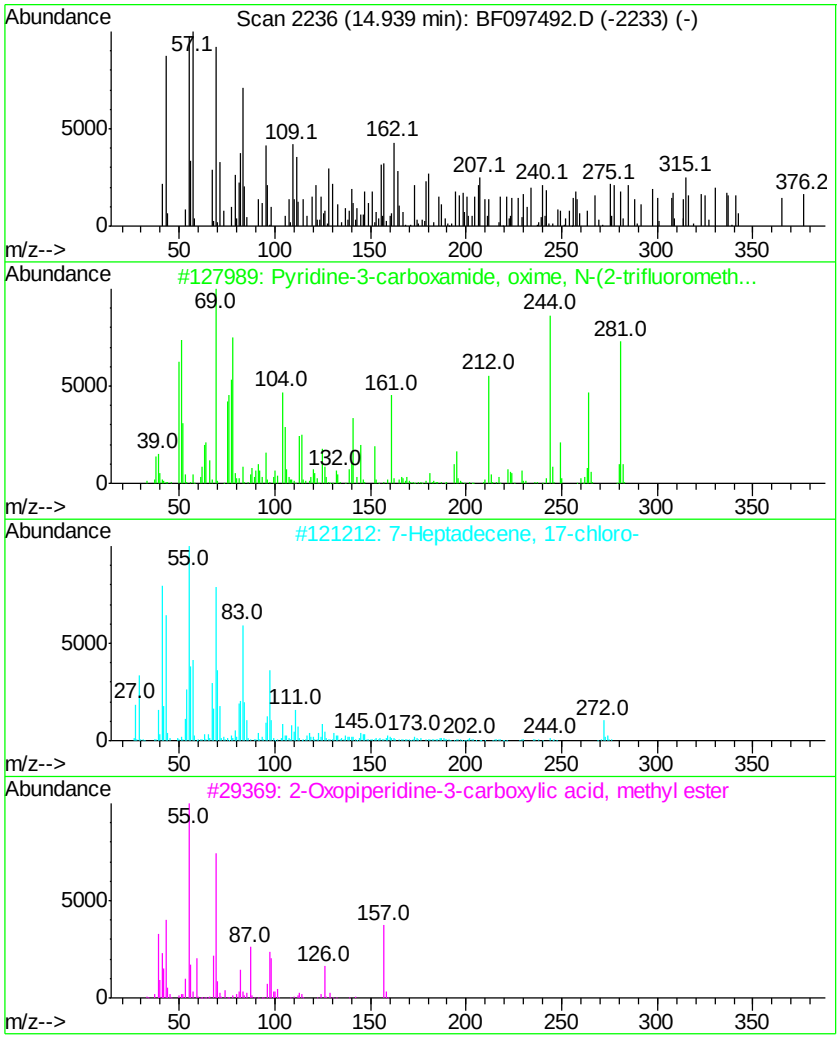
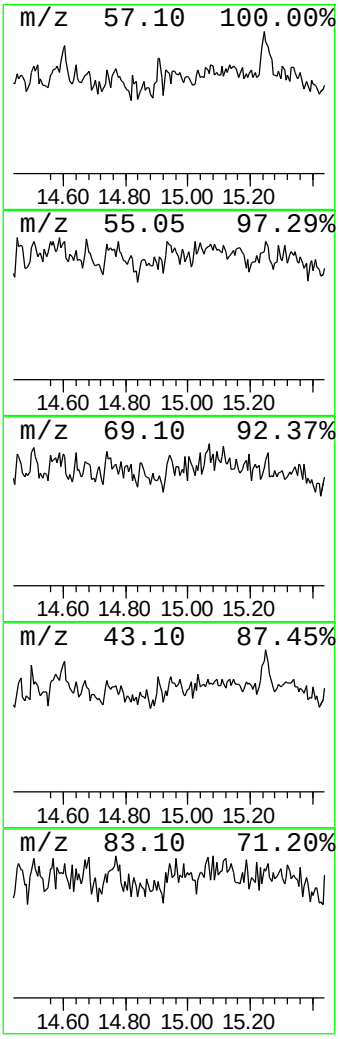
Peak Number 10 Pyridine-3-carboxamide, oxi... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	5.38 ng	116954	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-3-carboxamide, oxime, N...	281	C13H10F3N3O	288246-53-7	68
2	7-Heptadecene, 17-chloro-	272	C17H33Cl	056554-79-1	35
3	2-Oxopiperidine-3-carboxylic aci...	157	C7H11NO3	1000303-46-8	27
4	1,22-Docosanediol	342	C22H46O2	022513-81-1	25
5	10-Nonadecanol	284	C19H40O	016840-84-9	16





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Data File : BF097492.D
Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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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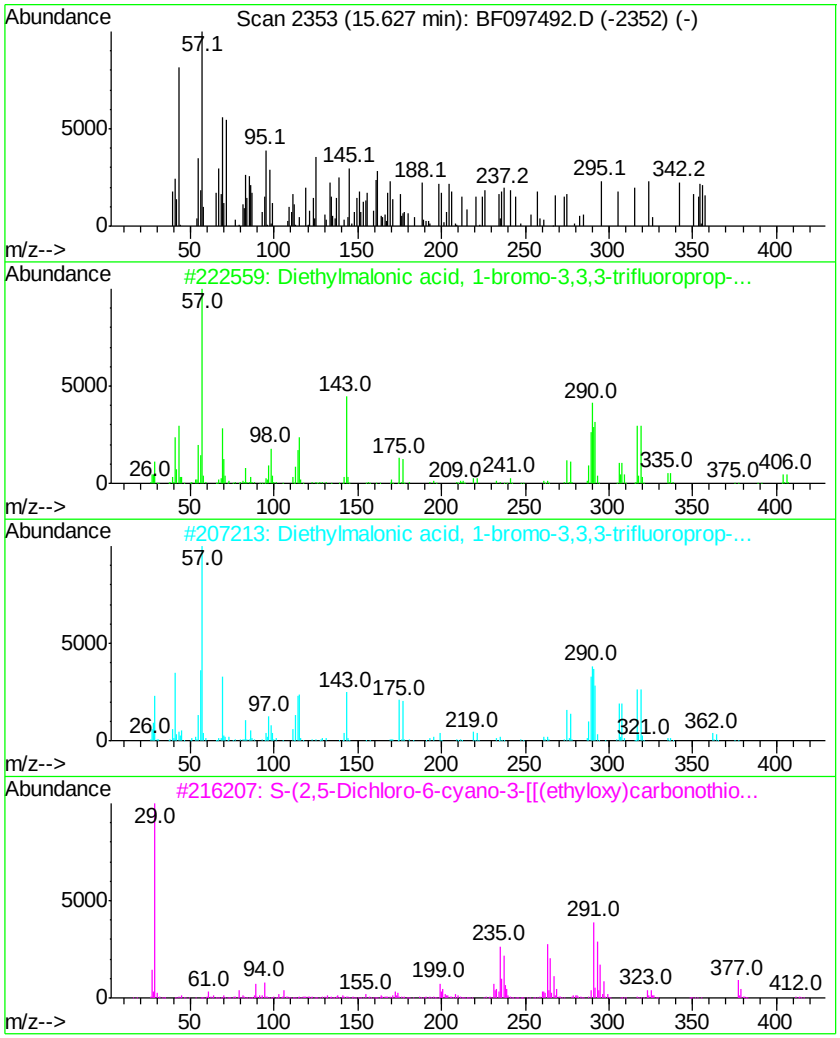
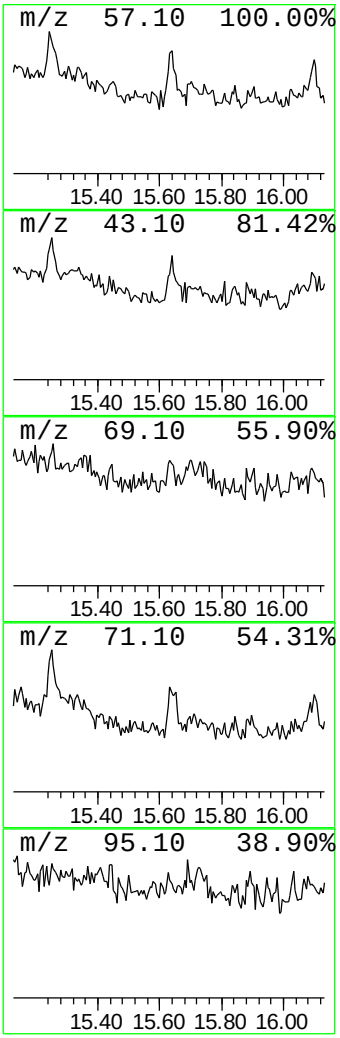
Peak Number 11 unknown15.63 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	2.66 ng	57797	Perylene-d12	14.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylmalonic acid, 1-bromo-3,3...	432	C17H28BrF3O4	1000370-79-9	12
2	Diethylmalonic acid, 1-bromo-3,3...	390	C14H22BrF3O4	1000370-79-5	12
3	S-(2,5-Dichloro-6-cyano-3-[[(eth...	412	C12H10Cl2N2O2S4	194228-14-3	9
4	Dibutyltin dibromide	392	C8H18Br2Sn	000996-08-7	8
5	Decanedioic acid, 2,9-dibromo-, ...	414	C14H24Br2O4	000868-71-3	7





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Data File : BF097492.D
Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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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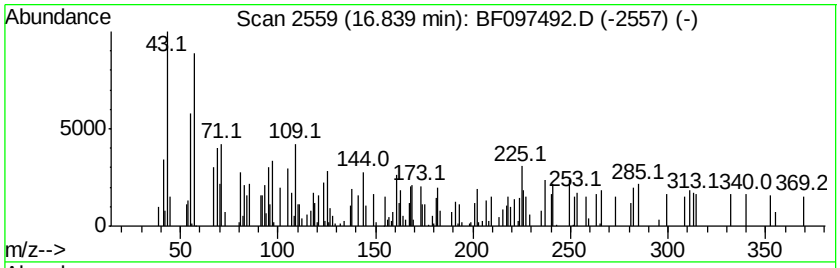
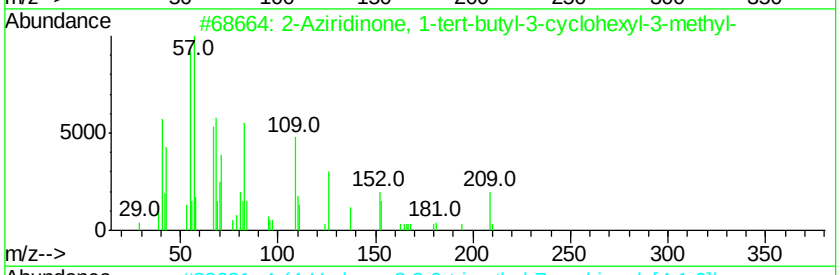
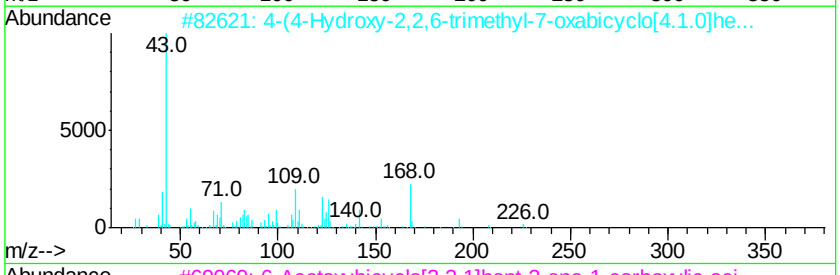
Peak Number 12 unknown16.84 Concentration Rank 9

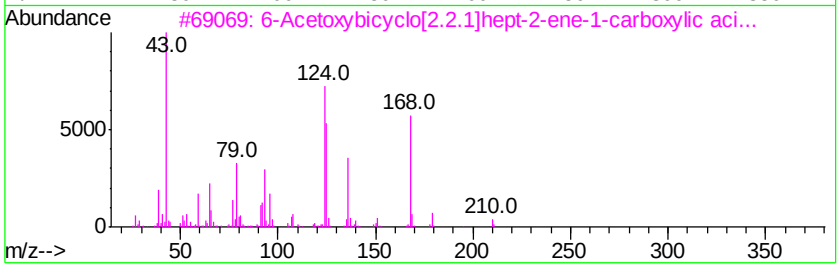
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	2.43 ng	52835	Perylene-d12	14.87

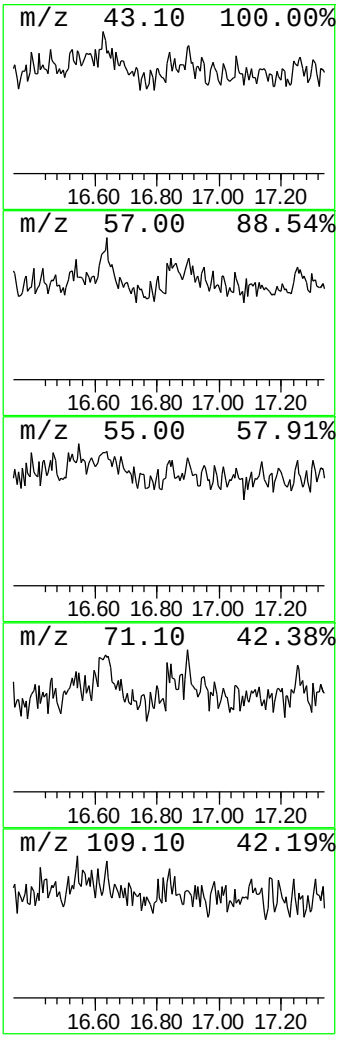
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Aziridinone, 1-tert-butyl-3-cy...	209	C13H23NO	027147-96-2	15
2	4-(4-Hydroxy-2,2,6-trimethyl-7-o...	226	C13H22O3	1000190-34-1	10
3	6-Acetoxybicyclo[2.2.1]hept-2-en...	210	C11H14O4	1000191-48-5	10
4	1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	10
5	2-Hydroxy-3-acetyl-6-methyl-4-py...	168	C8H8O4	1000322-41-6	10











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Data File : BF097492.D
Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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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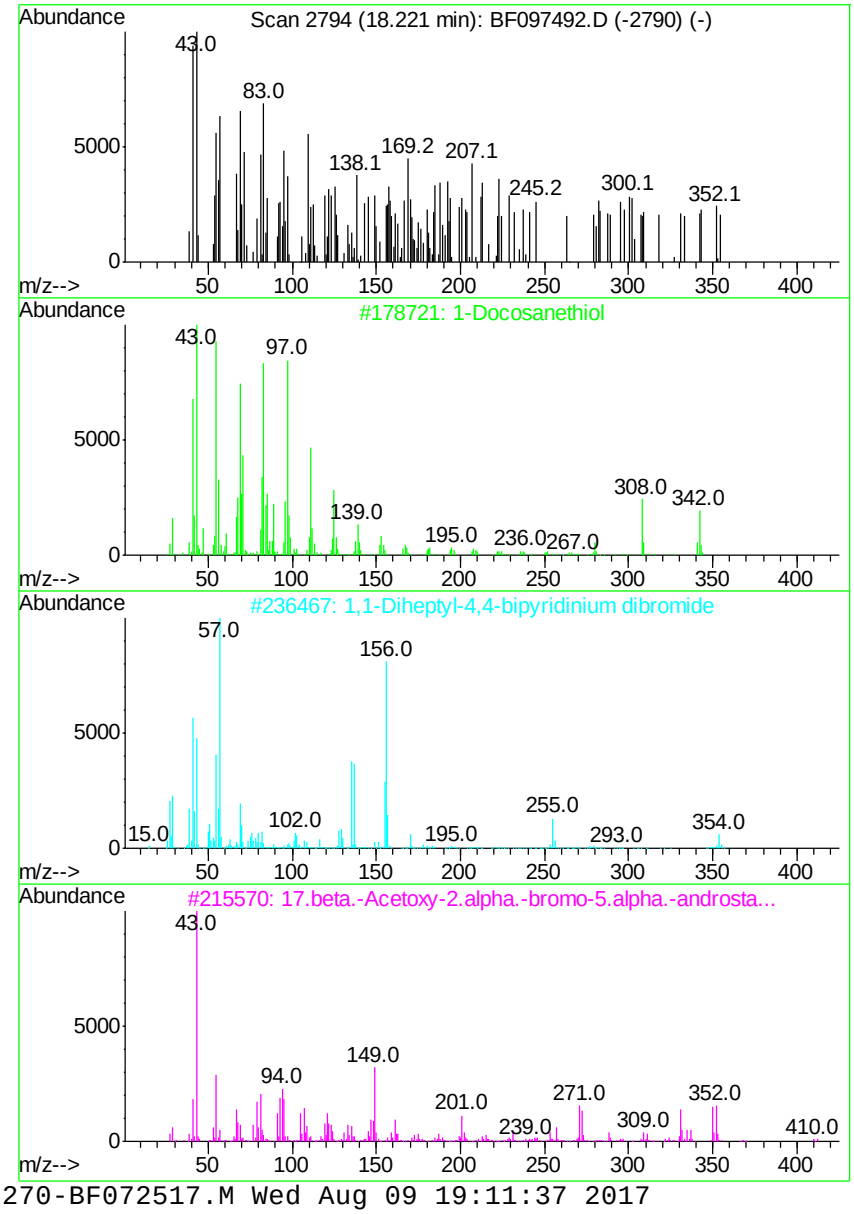
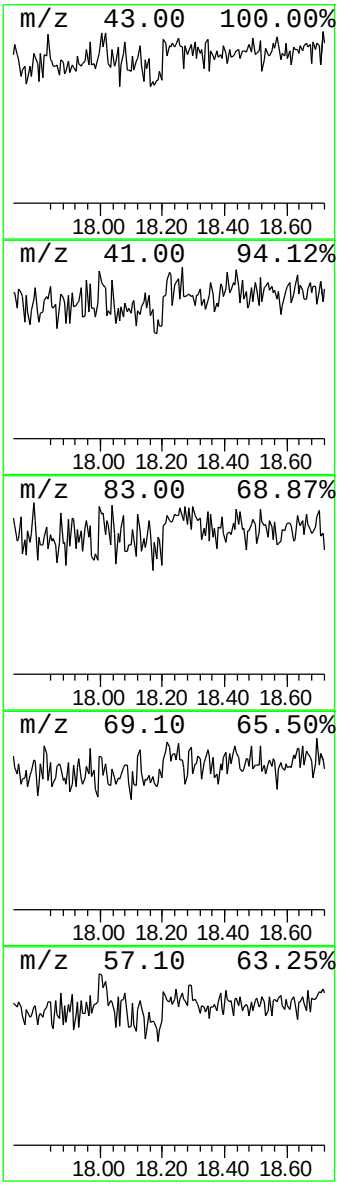
Peak Number 13 unknown18.22 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.22	4.91 ng	106864	Perylene-d12	14.87

Hit# of 3	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanethiol	342	C22H46S	007773-83-3	11
2	1,1-Diheptyl-4,4-bipyridinium di...	512	C24H38Br2N2	006159-05-3	2
3	17.beta.-Acetoxy-2.alpha.-bromo-...	410	C21H31BrO3	006173-35-9	1





Tentatively Identified Compound (LSC) summary

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Data File : BF097492.D
Acq On : 9 Aug 2017 2:19
Operator : SJ/JU
Sample : I4657-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-01-080717-B

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.54	6.4	ng	220384	1	6.40	684343	20.0
unknown6.18	6.18	62.9	ng	2150670	1	6.40	684343	20.0
n-Hexadecanoic acid	11.47	2.9	ng	97391	4	10.90	664150	20.0
Decanoic acid, si...	12.24	2.2	ng	77731	5	13.53	708625	20.0
17-Pentatriacontene	13.43	2.2	ng	79528	5	13.53	708625	20.0
unknown13.63	13.63	2.2	ng	78812	5	13.53	708625	20.0
unknown14.38	14.38	3.9	ng	84536	6	14.87	435177	20.0
unknown14.46	14.46	2.4	ng	52694	6	14.87	435177	20.0
Pyridine-3-carbox...	14.94	5.4	ng	116954	6	14.87	435177	20.0
unknown15.63	15.63	2.7	ng	57797	6	14.87	435177	20.0
unknown16.84	16.84	2.4	ng	52835	6	14.87	435177	20.0
unknown18.22	18.22	4.9	ng	106864	6	14.87	435177	20.0