LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086882.D
Acq On : 11 May 2016 5:41
Operator : UM/SJ
Sample : H2916-04
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

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-BF050916.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	3.173	93	95	101	rBV	17288	38141	1.87%	0.177%
2	3.436	114	118	123	rBV	129558	279552	13.69%	1.295%
3	4.819	237	239	248	rBV	86826	153824	7.53%	0.713%
4	5.276	277	279	295	rBV	784063	951845	46.62%	4.410%
5	5.676	310	314	318	rBV2	12852	35576	1.74%	0.165%
6	6.339	370	372	380	rBV	792744	1170697	57.34%	5.423%
7	6.453	380	382	390	rVB	1006113	1167253	57.17%	5.407%
8	6.682	400	402	413	rVB	1126179	1011949	49.57%	4.688%
9	6.842	413	416	418	rBV	617282	814622	39.90%	3.774%
10	6.944	423	425	430	rVB	22901	27368	1.34%	0.127%
11	7.253	450	452	462	rBV	756255	748386	36.66%	3.467%
12	7.973	512	515	519	rBV2	1202852	1589492	77.86%	7.363%
13	8.042	519	521	527	rVB	26260	36993	1.81%	0.171%
14	8.682	575	577	583	rVB	98304	92637	4.54%	0.429%
15	8.785	583	586	588	rBV	48278	54756	2.68%	0.254%
16	9.048	606	609	611	rBV	1973023	1631883	79.93%	7.560%
17	9.150	614	618	619	rVV2	31129	54269	2.66%	0.251%
18	9.379	636	638	640	rBV2	27928	37686	1.85%	0.175%
19	9.448	642	644	647	rVV	202643	194939	9.55%	0.903%
20	9.505	647	649	651	rVB3	12263	21291	1.04%	0.099%
21	9.585	653	656	658	rVV	60477	75747	3.71%	0.351%
22	9.665	661	663	665	rBV	77581	86501	4.24%	0.401%
23	9.722	665	668	669	rVV	1037943	1096668	53.72%	5.080%
24	9.745	669	670	673	rVB	88107	109621	5.37%	0.508%
25	9.893	680	683	684	rBV	18410	28031	1.37%	0.130%
26	9.916	684	685	687	rVV2	22397	31859	1.56%	0.148%
27	9.985	687	691	692	rVV3	24450	49208	2.41%	0.228%
28	10.019	692	694	697	rVV	13997	23224	1.14%	0.108%
29	10.156	704	706	708	rBV	156109	124992	6.12%	0.579%
30	10.259	714	715	719	rVB	66832	95643	4.68%	0.443%
31	10.373	722	725	728	rBV	63071	89916	4.40%	0.417%
32	10.511	734	737	739	rBV2	888345	1273378	62.37%	5.899%
33	10.625	746	747	751	rBV	152630	208580	10.22%	0.966%
34	10.819	761	764	766	rBV2	25975	46139	2.26%	0.214%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H2916-04
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

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

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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.071	785	786	787	rBV	71839	73014	3.58%	0.338%
36	11.093	787	788	792	rVB2	47098	70459	3.45%	0.326%
37	11.196	795	797	798	rBV	1075337	960845	47.06%	4.451%
38	11.276	801	804	806	rVB	101448	134411	6.58%	0.623%
39	11.494	821	823	825	rBV	33362	37409	1.83%	0.173%
40	11.699	839	841	842	rBV	42070	40655	1.99%	0.188%
41	11.734	842	844	846	rVV2	53710	103312	5.06%	0.479%
42	11.802	849	850	855	rVV	87056	137007	6.71%	0.635%
43	11.996	865	867	871	rVB	40600	49931	2.45%	0.231%
44	12.248	887	889	890	rBV	20344	25836	1.27%	0.120%
45	12.294	890	893	895	rVB4	18347	37519	1.84%	0.174%
46	12.396	900	902	905	rBV	195639	269131	13.18%	1.247%
47	12.499	909	911	912	rBV	59562	54783	2.68%	0.254%
48	12.625	919	922	924	rBV	377353	406847	19.93%	1.885%
49	12.682	926	927	930	rVB2	30297	33220	1.63%	0.154%
50	12.774	933	935	938	rBV	1807876	2041578	100.00%	9.458%
51	12.957	947	951	954	rBV	33458	49770	2.44%	0.231%
52	13.025	954	957	959	rBV2	37550	46711	2.29%	0.216%
53	13.059	959	960	964	rVB	25356	25554	1.25%	0.118%
54	13.151	964	968	969	rBV	21329	35780	1.75%	0.166%
55	13.185	969	971	974	rVB	18149	21360	1.05%	0.099%
56	13.311	981	982	984	rBV	27261	23229	1.14%	0.108%
57	13.619	1006	1009	1012	rVB2	18839	37602	1.84%	0.174%
58	13.711	1012	1017	1024	rBV2	55951	198846	9.74%	0.921%
59	13.825	1024	1027	1028	rBV2	795111	954715	46.76%	4.423%
60	13.997	1039	1042	1044	rVB	18683	25271	1.24%	0.117%
61	14.305	1067	1069	1070	rBV	25859	28238	1.38%	0.131%
62	14.351	1070	1073	1077	rVV3	12690	29656	1.45%	0.137%
63	14.591	1092	1094	1098	rVB2	13785	21323	1.04%	0.099%
64	14.660	1098	1100	1103	rBV2	20307	31098	1.52%	0.144%
65	14.820	1112	1114	1119	rBV	70617	142996	7.00%	0.662%
66	14.900	1119	1121	1122	rBV	14934	28031	1.37%	0.130%
67	15.048	1131	1134	1136	rBV2	18698	31514	1.54%	0.146%
68	15.082	1136	1137	1140	rVV	44540	66435	3.25%	0.308%
69	15.140	1140	1142	1145	rVV	88883	116396	5.70%	0.539%
70	15.197	1145	1147	1155	rVB	597954	720940	35.31%	3.340%
71	15.482	1169	1172	1174	rVB	32137	53643	2.63%	0.249%

LSC Area Percent Report

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Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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72	15.608	1180	1183	1186	rBV	19327	33610	1.65%	0.156%
73	15.974	1212	1215	1219	rBV	57289	111663	5.47%	0.517%
74	16.043	1219	1221	1224	rVB2	16173	24458	1.20%	0.113%
75	16.488	1257	1260	1263	rBV	23454	51683	2.53%	0.239%
76	16.580	1263	1268	1272	rVB2	72130	191198	9.37%	0.886%
77	16.865	1290	1293	1300	rVB	24796	62157	3.04%	0.288%
78	17.311	1328	1332	1338	rBV2	70124	204302	10.01%	0.946%
79	18.214	1405	1411	1420	rVB2	49453	191921	9.40%	0.889%
80	19.323	1503	1508	1515	rVB5	22340	97490	4.78%	0.452%

Sum of corrected areas: 21586213

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Misc :
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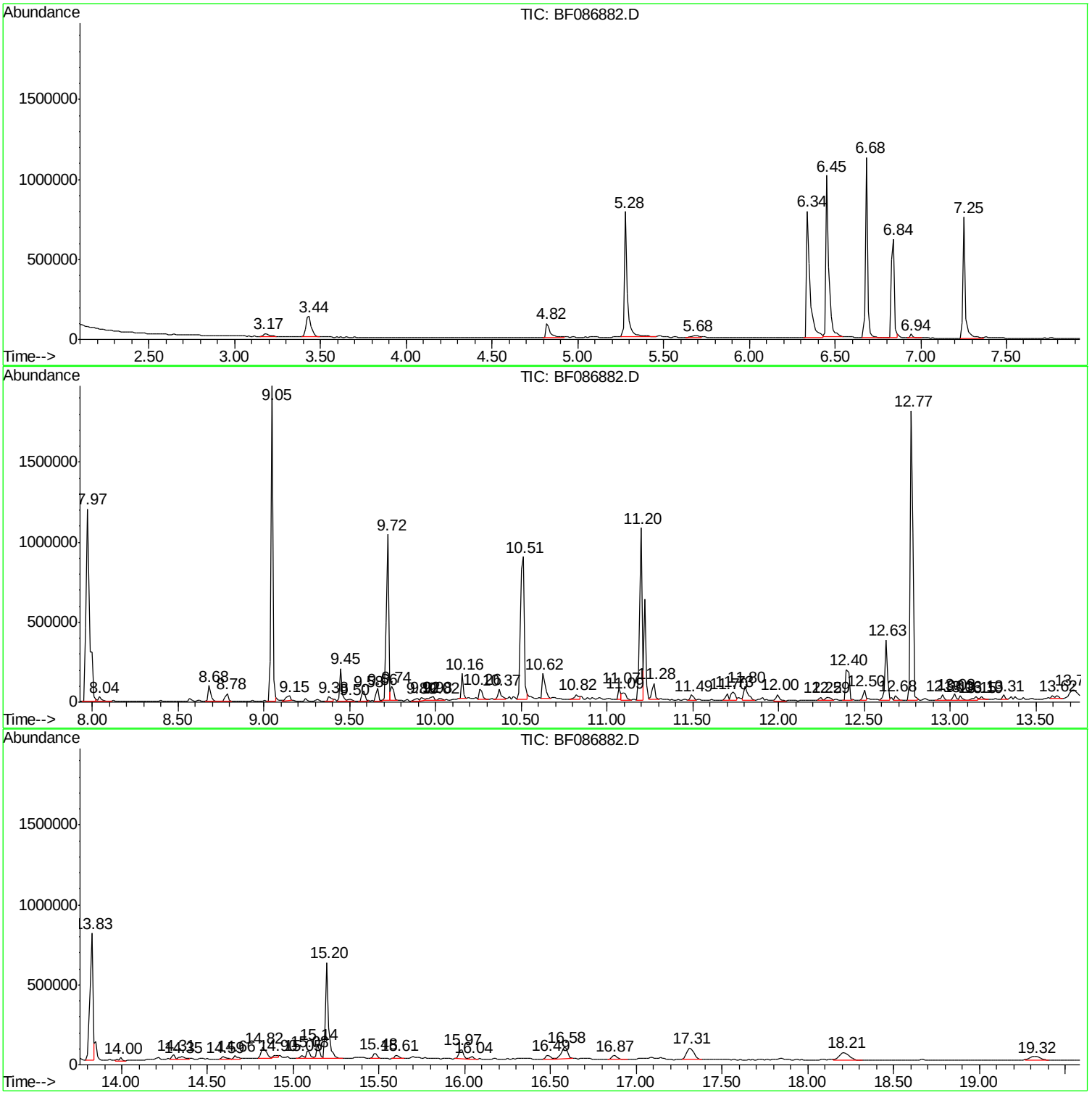
Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086882.D
Acq On : 11 May 2016 5:41
Operator : UM/SJ
Sample : H2916-04
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

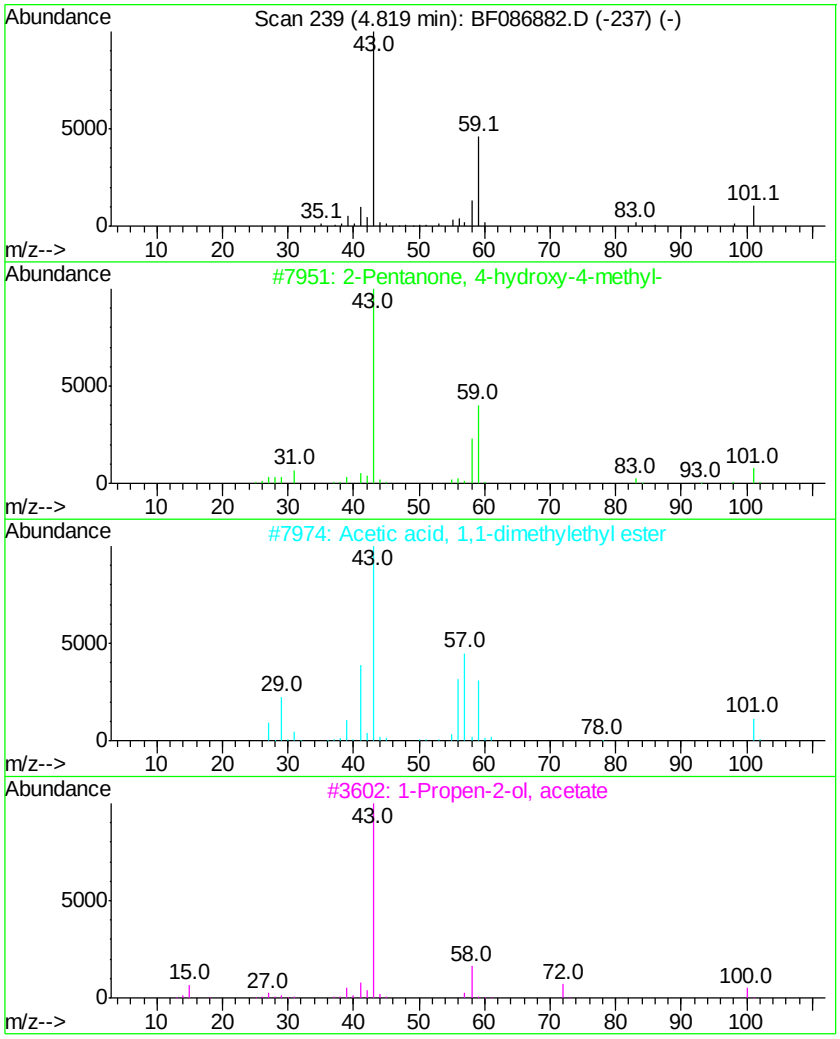
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

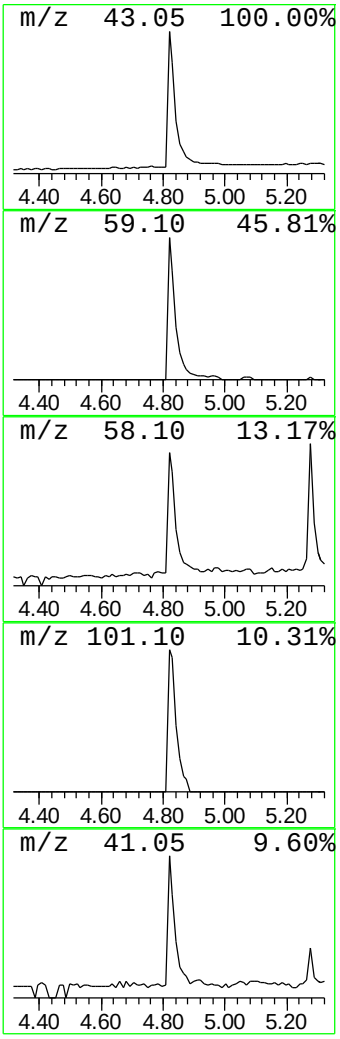
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	3.04 ng	153824	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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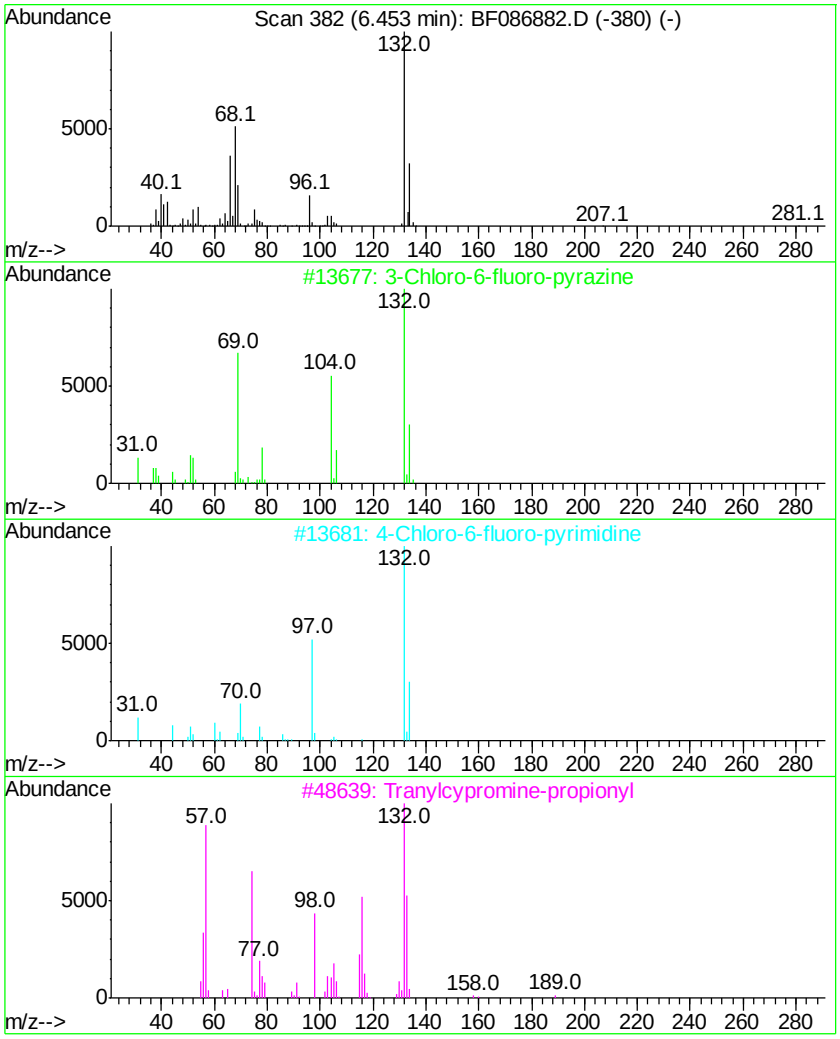
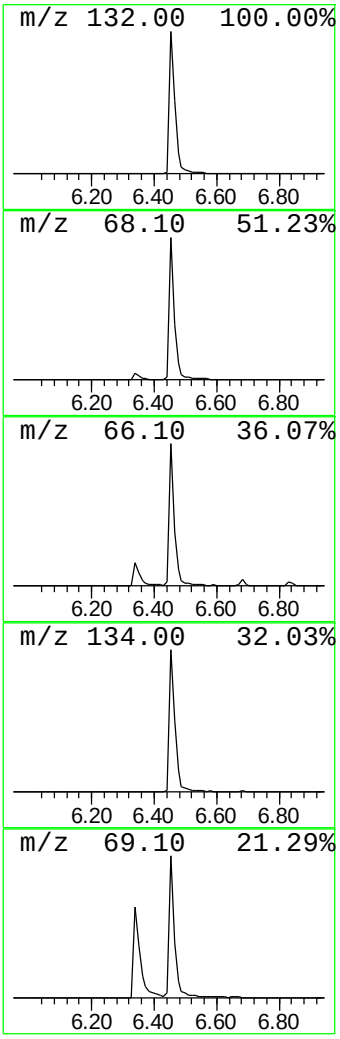
Peak Number 3 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	23.07 ng	1167250	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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TIC Library : C:\DATABASE\NIST02.L
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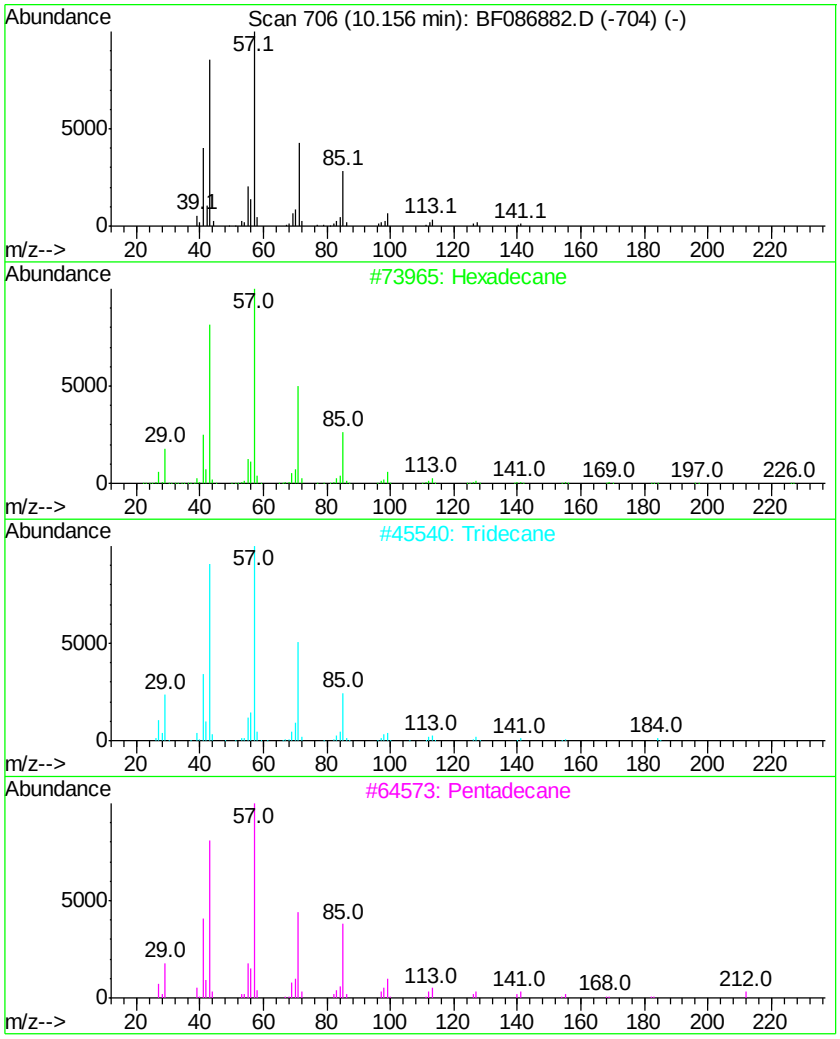
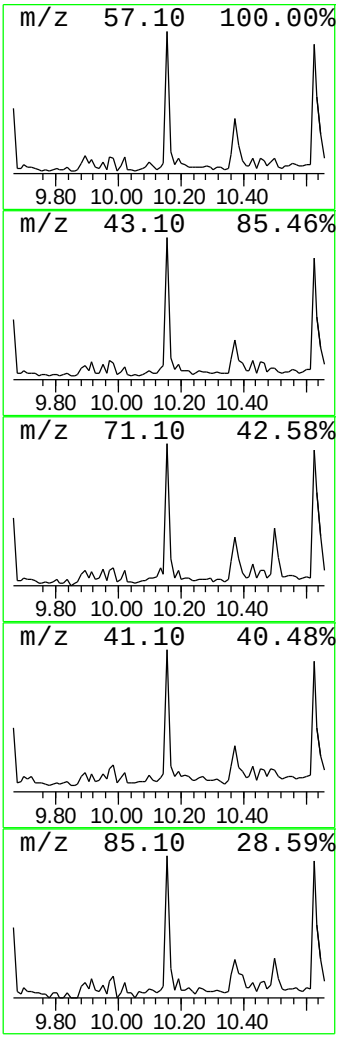
****

Peak Number 5 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	2.28 ng	124992	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tridecane	184	C13H28	000629-50-5	90
3	Pentadecane	212	C15H32	000629-62-9	86
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	86
5	Eicosane	282	C20H42	000112-95-8	72





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TIC Library : C:\DATABASE\NIST02.L
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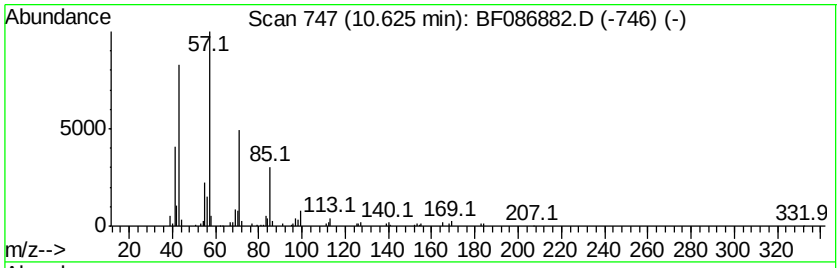
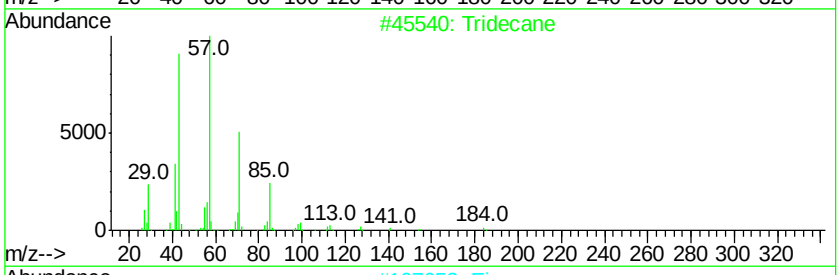
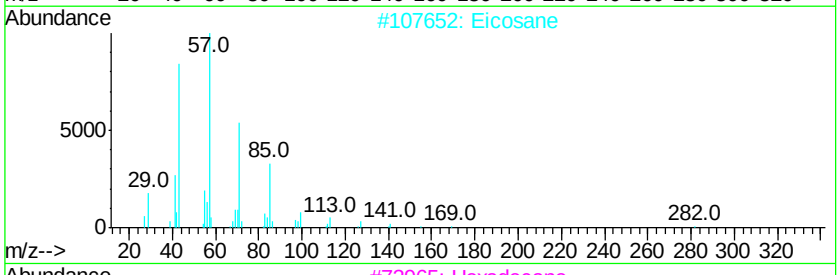
Peak Number 6 Tridecane Concentration Rank 7

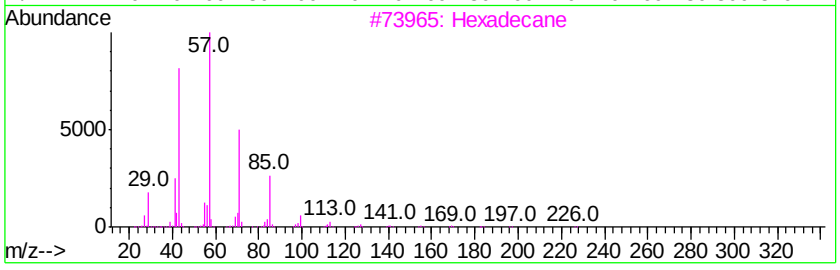
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	4.34 ng	208580	Phenanthrene-d10	11.20

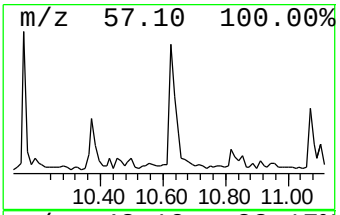
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Hexadecane	226	C16H34	000544-76-3	91
4	Octadecane	254	C18H38	000593-45-3	90
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	86

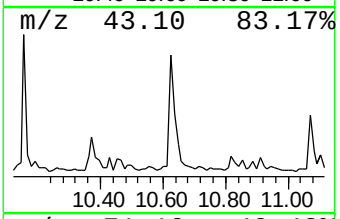


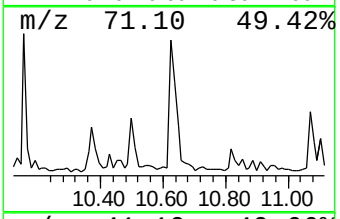


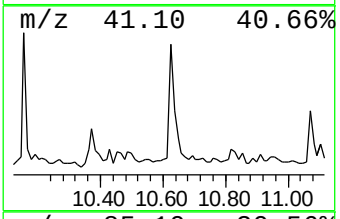


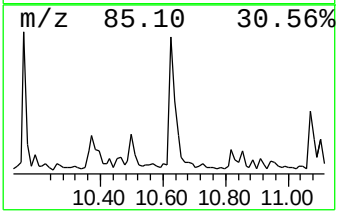












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

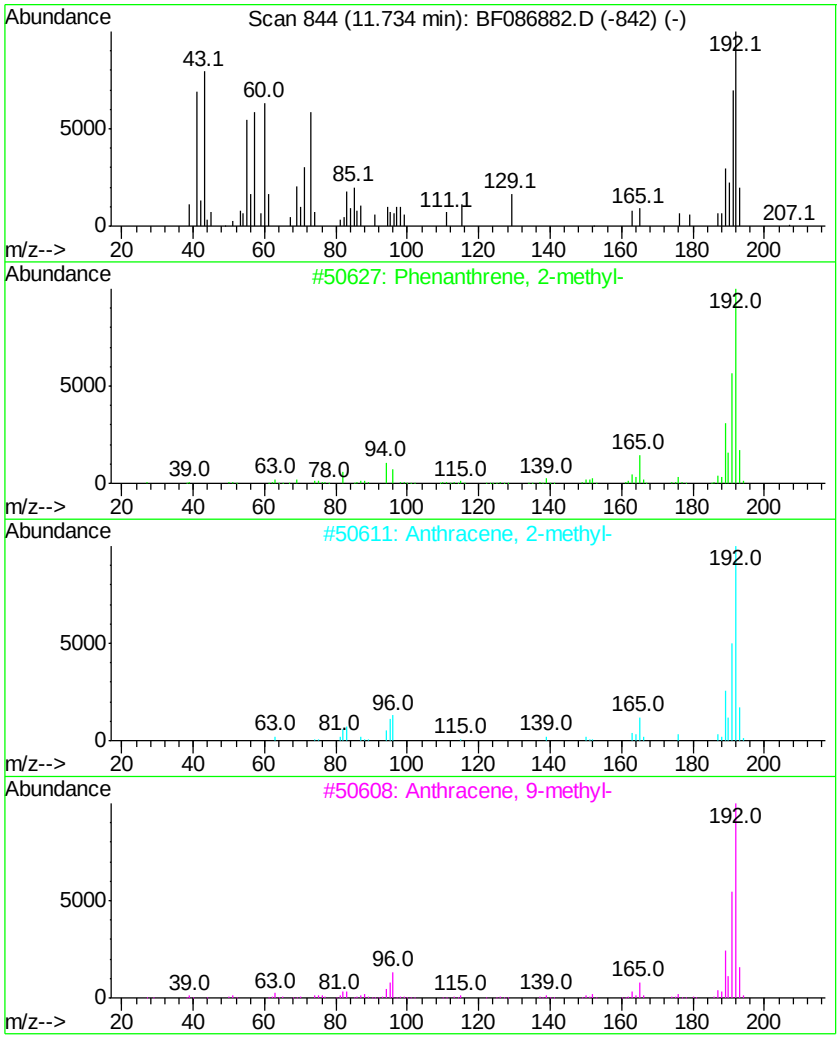
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

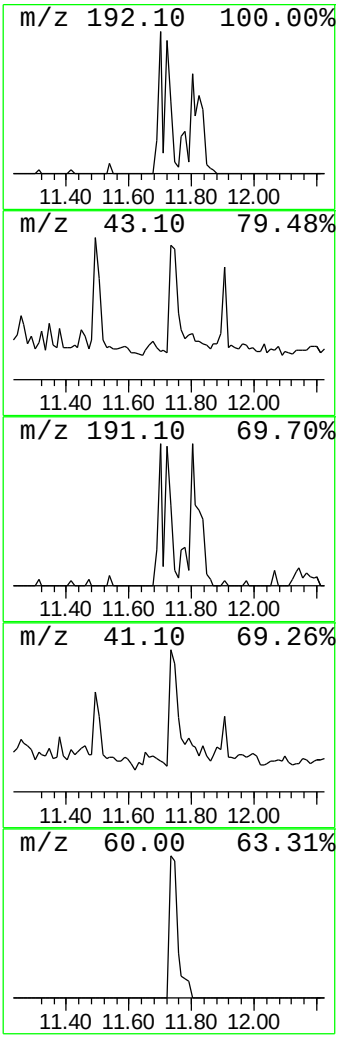
****

Peak Number 7 Phenanthrene, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	2.15 ng	103312	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	55
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	50
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	49
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	47
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	46





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Data File : BF086882.D
Acq On : 11 May 2016 5:41
Operator : UM/SJ
Sample : H2916-04
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

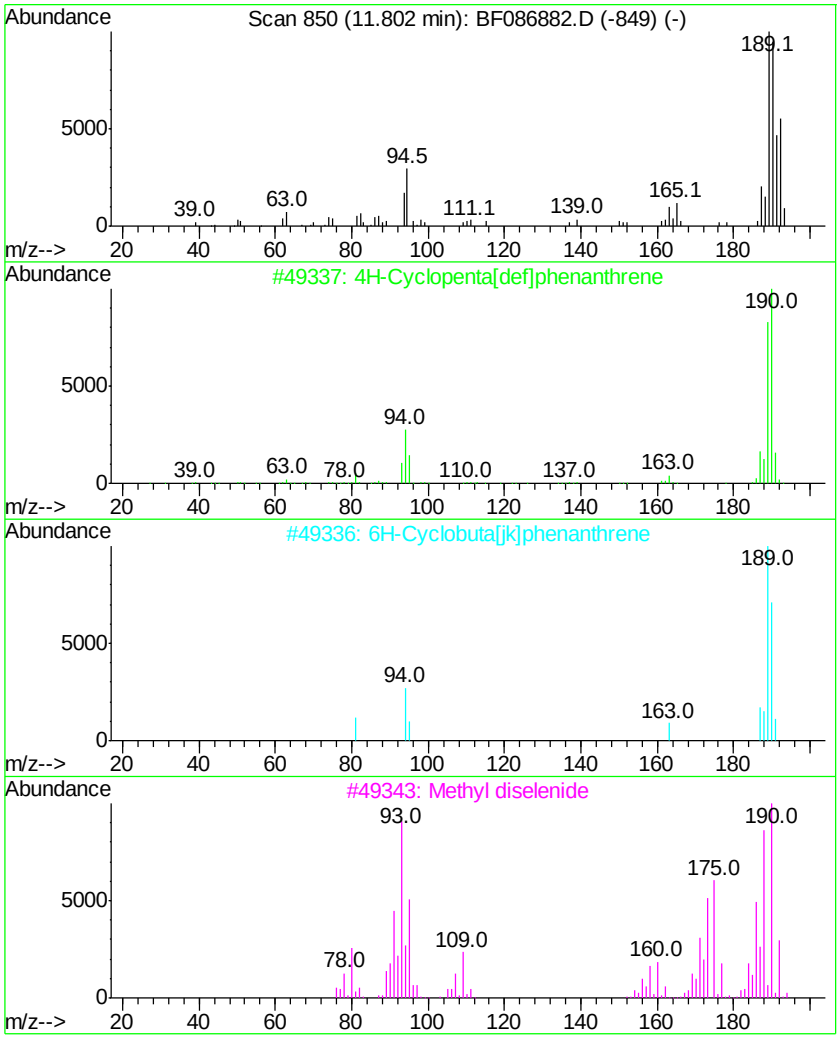
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

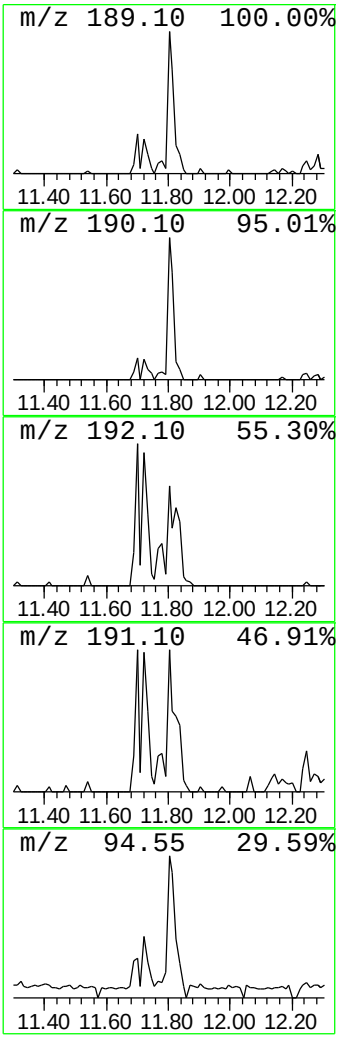
****

Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.85 ng	137007	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	38
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	18
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	18





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Acq On : 11 May 2016 5:41
Operator : UM/SJ
Sample : H2916-04
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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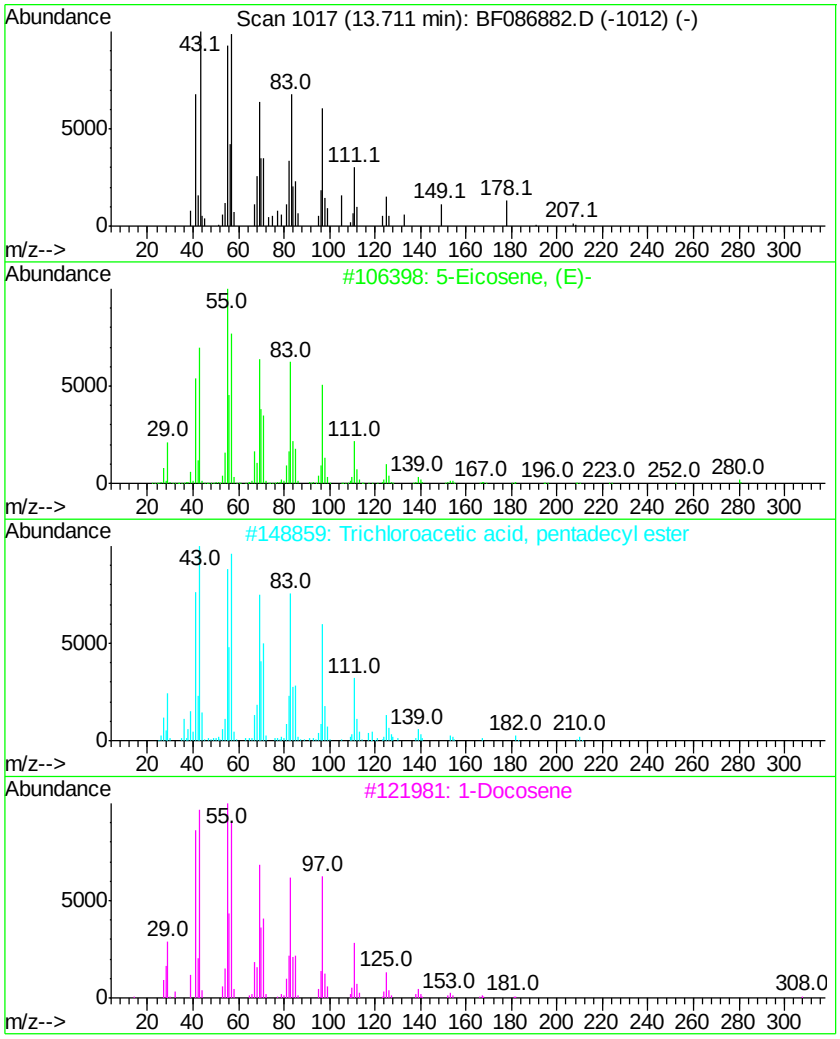
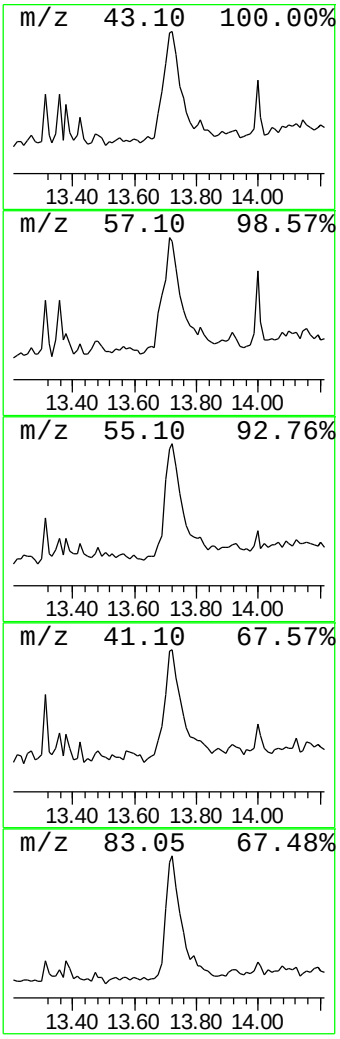
Peak Number 9 5-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	4.17 ng	198846	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3	1-Docosene	308	C22H44	001599-67-3	90
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87





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Acq On : 11 May 2016 5:41
Operator : UM/SJ
Sample : H2916-04
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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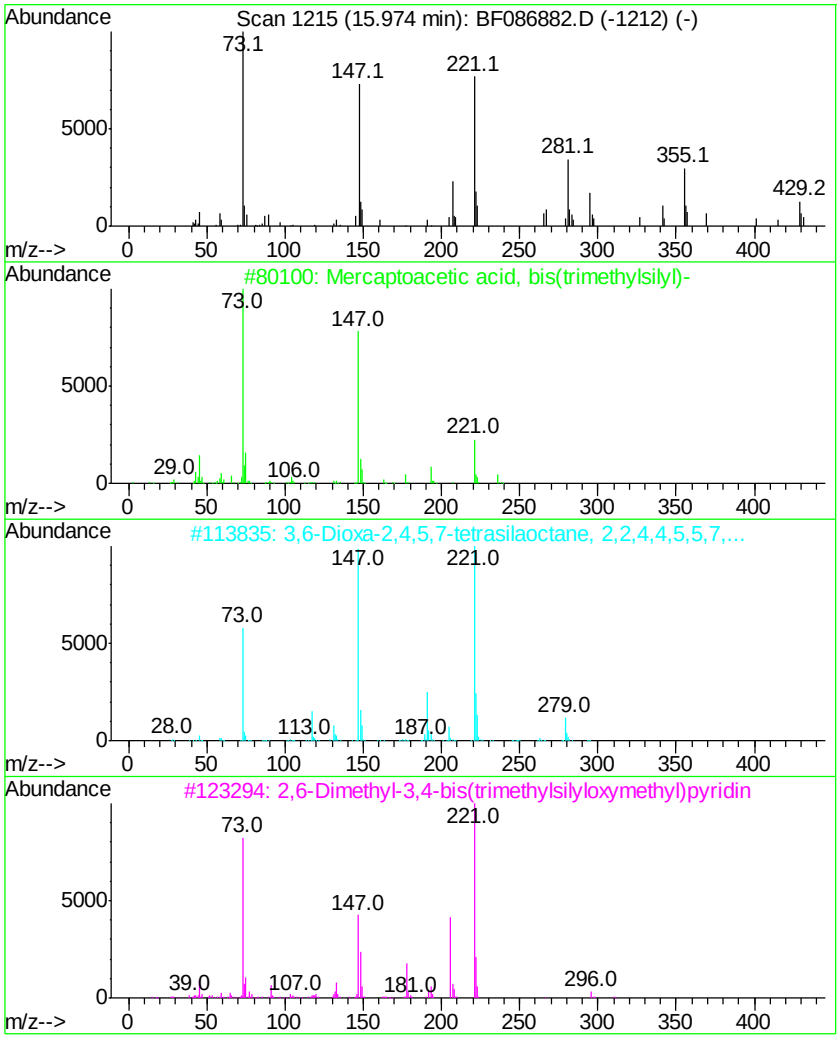
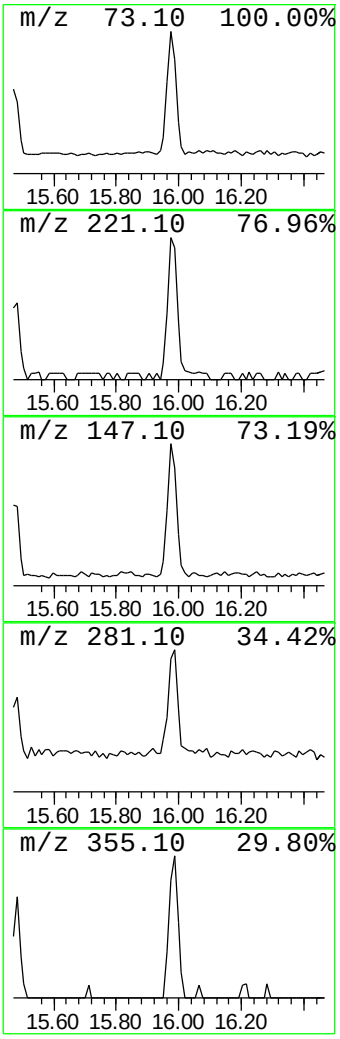
Peak Number 10 unknown15.97 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	3.10 ng	111663	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	40
2	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
3	2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29NO2Si2	1000079-52-1	32
4	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	32
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	27





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Sample : H2916-04
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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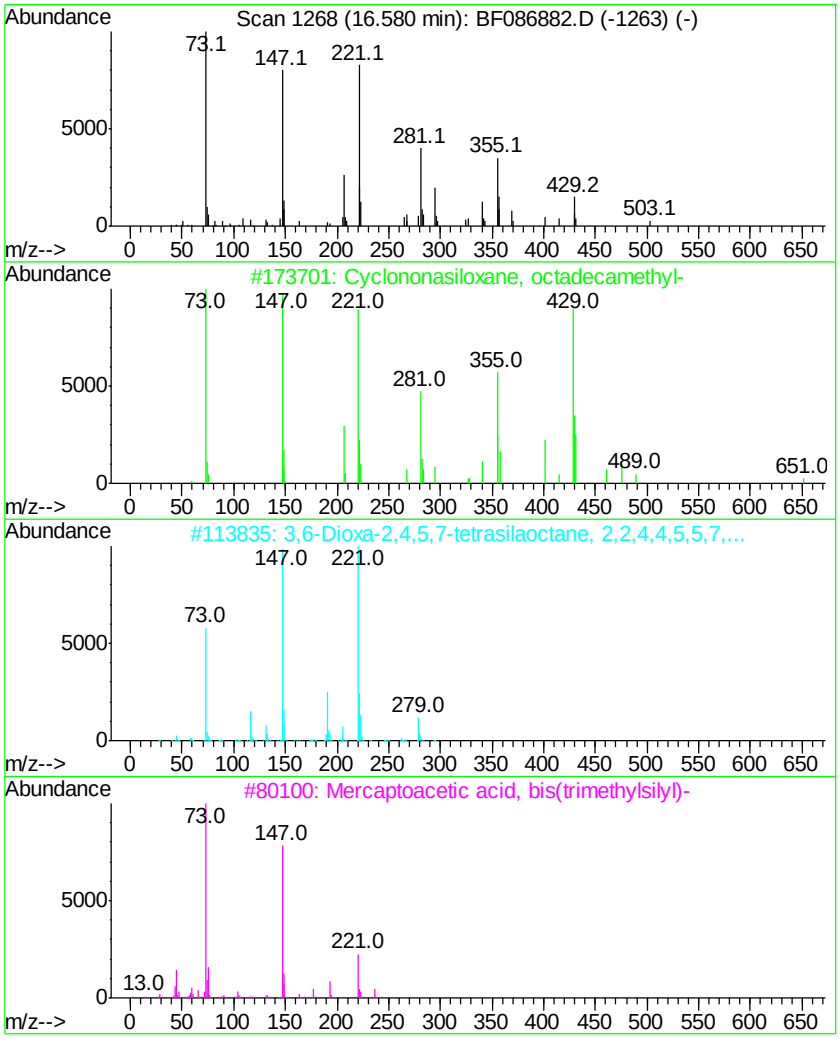
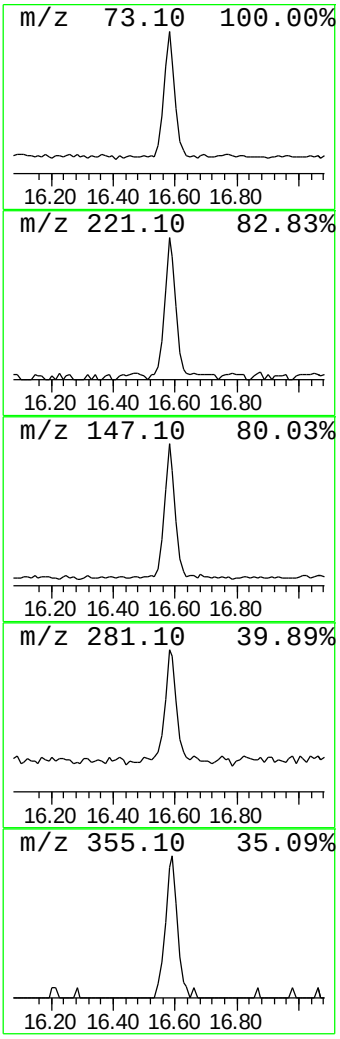
Peak Number 11 Cyclononasiloxane, octadeca... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.58	5.30 ng	191198	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
2	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	40
3	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	38
4	Dithioerythritol, O,O',S,S'-tetr...	442	C16H42O2S2Si4	1000079-30-7	32
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	30





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086882.D
Acq On : 11 May 2016 5:41
Operator : UM/SJ
Sample : H2916-04
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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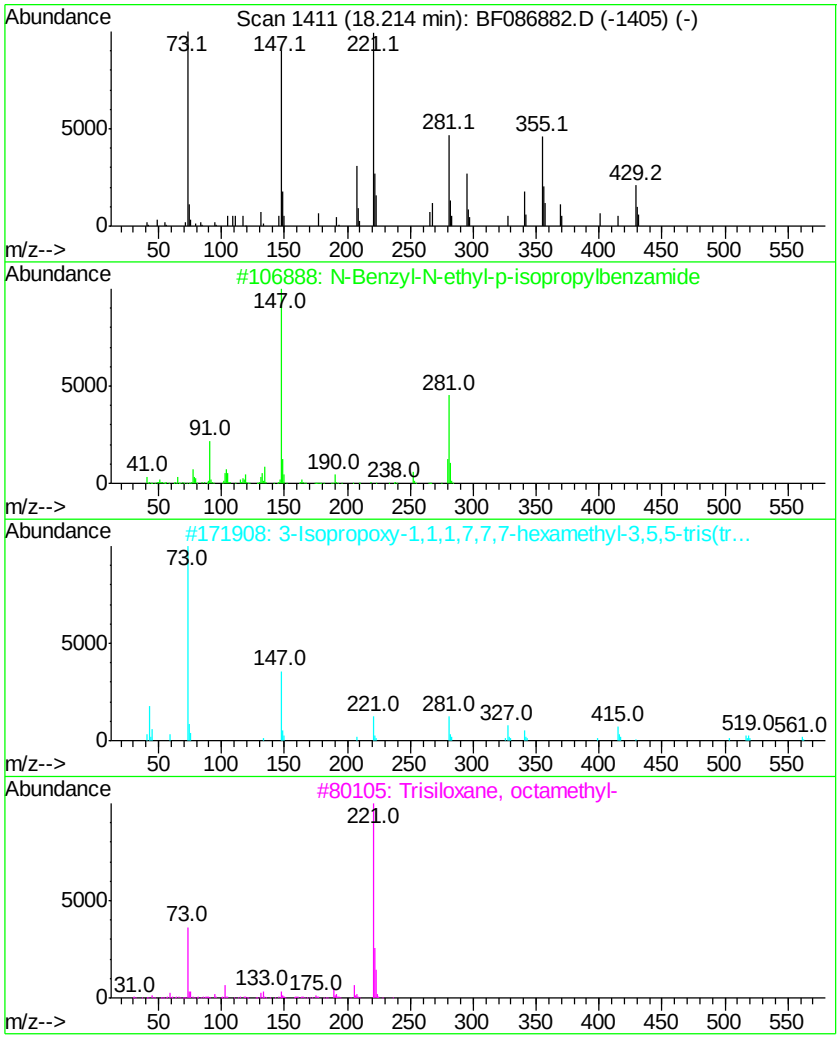
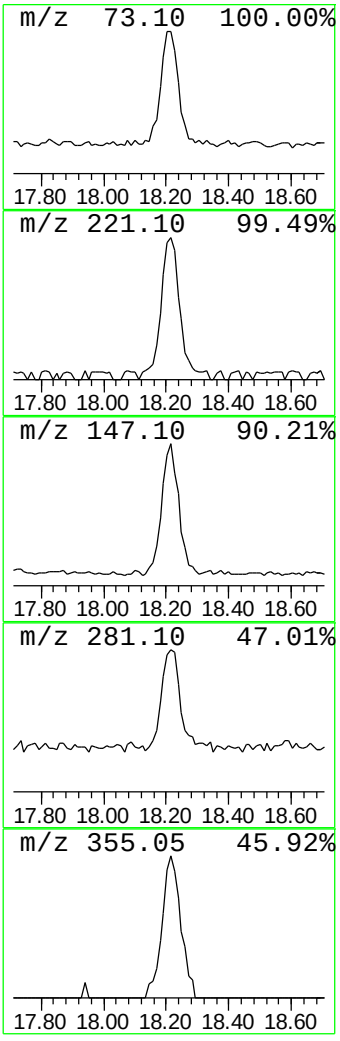
Peak Number 13 unknown18.21 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.21	5.32 ng	191921	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22
2	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	16
3	Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	14
4	2-(2',4',4',6',6',8',8'-Heptamet...	652	C16H48O10Si9	145344-72-5	12
5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	12





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Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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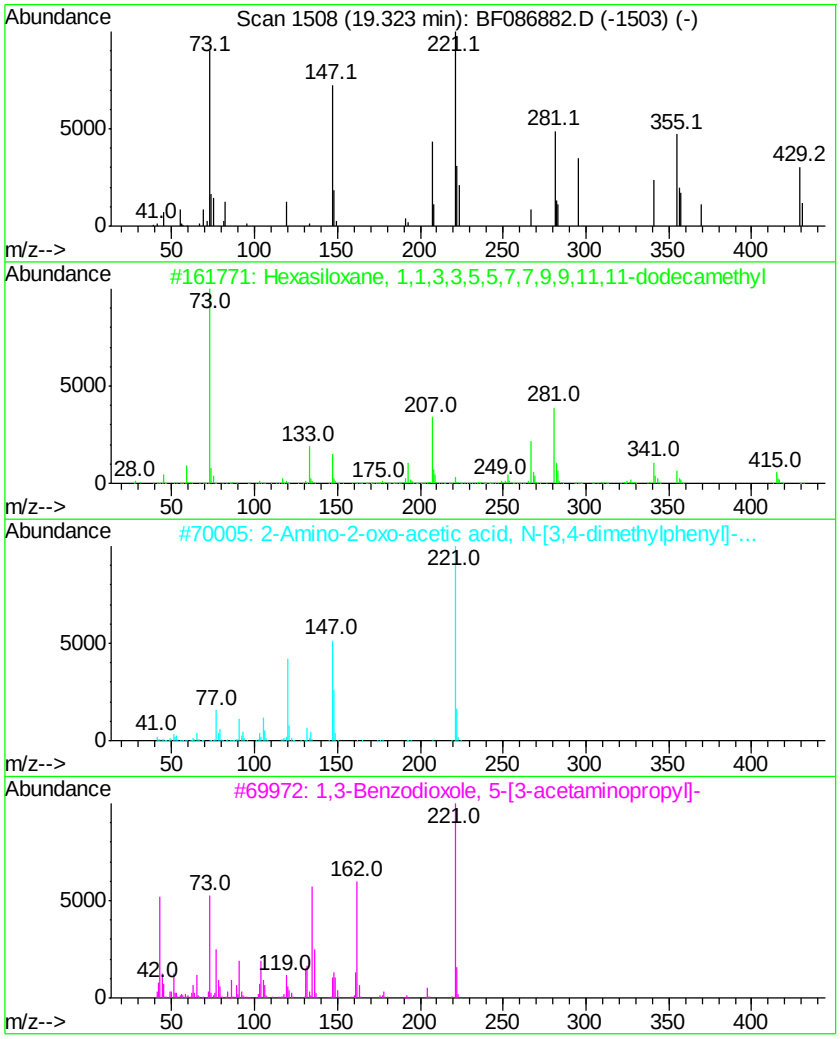
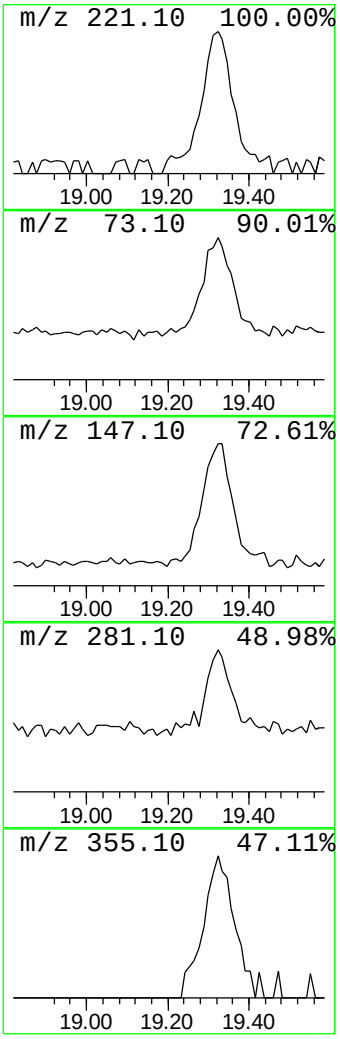
Peak Number 14 unknown19.32 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	2.70 ng	97490	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, 1,1,3,3,5,5,7,7,9,...	430	C12H38O5Si6	000995-82-4	10
2	2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	9
3	1,3-Benzodioxole, 5-[3-acetamino...	221	C12H15NO3	1000124-33-0	9
4	9-(Methylaminomethyl)anthracene	221	C16H15N	073356-19-1	9
5	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
Data File : BF086882.D
Acq On : 11 May 2016 5:41
Operator : UM/SJ
Sample : H2916-04
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-4K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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
2-Pentanone, 4-hy...	4.82	3.0	ng	153824	1	6.68	1011950	20.0
unknown6.45	6.45	23.1	ng	1167250	1	6.68	1011950	20.0
Hexadecane	10.16	2.3	ng	124992	3	9.72	1096670	20.0
Tridecane	10.62	4.3	ng	208580	4	11.20	960845	20.0
Phenanthrene, 2-m...	11.73	2.1	ng	103312	4	11.20	960845	20.0
4H-Cyclopenta[def...	11.80	2.9	ng	137007	4	11.20	960845	20.0
5-Eicosene, (E)-	13.71	4.2	ng	198846	5	13.83	954715	20.0
unknown15.97	15.97	3.1	ng	111663	6	15.20	720940	20.0
Cyclononasiloxane...	16.58	5.3	ng	191198	6	15.20	720940	20.0
unknown18.21	18.21	5.3	ng	191921	6	15.20	720940	20.0
unknown19.32	19.32	2.7	ng	97490	6	15.20	720940	20.0