LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050416\
Data File : BF086696.D
Acq On : 5 May 2016 00:28
Operator : UM/SJ
Sample : H2715-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

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-BF050416.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	4.921	246	248	254	rBV	99044	184200	3.45%	0.414%
2	5.333	281	284	286	rBV	4820769	5027483	94.20%	11.296%
3	6.384	373	376	379	rBV	4288367	4915756	92.10%	11.045%
4	6.510	384	387	389	rBV	5189779	5337131	100.00%	11.991%
5	6.739	405	407	409	rBV	1206758	1068253	20.02%	2.400%
6	6.899	418	421	423	rBV	3538494	3836612	71.89%	8.620%
7	7.310	454	457	459	rBV	3218223	3513696	65.83%	7.894%
8	7.413	465	466	473	rVB	37717	59814	1.12%	0.134%
9	8.019	517	519	525	rBV	871006	1317808	24.69%	2.961%
10	9.105	611	614	616	rBV	4460037	4040369	75.70%	9.078%
11	9.196	619	622	630	rVB5	26141	86843	1.63%	0.195%
12	9.493	646	648	651	rBV	377640	488974	9.16%	1.099%
13	9.722	666	668	670	rBV	82105	81486	1.53%	0.183%
14	9.779	670	673	674	rVV	1077938	1135168	21.27%	2.550%
15	9.802	674	675	679	rVB	76060	92963	1.74%	0.209%
16	9.973	689	690	692	rBV2	39019	55757	1.04%	0.125%
17	10.076	697	699	702	rBV2	26354	62229	1.17%	0.140%
18	10.213	709	711	713	rVB	119464	136121	2.55%	0.306%
19	10.316	719	720	724	rBV	65504	81946	1.54%	0.184%
20	10.431	727	730	733	rBV2	59353	115826	2.17%	0.260%
21	10.568	739	742	744	rBV	1836592	2339817	43.84%	5.257%
22	10.693	751	753	757	rVB	155152	226647	4.25%	0.509%
23	10.876	767	769	774	rVB4	24291	68133	1.28%	0.153%
24	11.139	790	792	797	rVB2	102982	192147	3.60%	0.432%
25	11.253	800	802	806	rBV2	859566	1378855	25.84%	3.098%
26	11.333	806	809	811	rVB	112204	142555	2.67%	0.320%
27	11.493	820	823	827	rBV3	43368	101220	1.90%	0.227%
28	11.756	844	846	847	rBV	72033	76593	1.44%	0.172%
29	11.791	847	849	851	rVV2	125631	191701	3.59%	0.431%
30	11.871	854	856	860	rVB2	91892	172756	3.24%	0.388%
31	11.974	860	865	866	rBV2	23932	61608	1.15%	0.138%
32	12.351	896	898	900	rVB	36084	56762	1.06%	0.128%
33	12.465	906	908	911	rBV	535510	486753	9.12%	1.094%
34	12.694	925	928	929	rBV	353276	478507	8.97%	1.075%

LSC Area Percent Report

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Sample : H2715-14
Misc :
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Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

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-BF050416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.728	929	931	935	rVB3	48647	102426	1.92%	0.230%
36	12.842	939	941	943	rVV	2807878	2684684	50.30%	6.032%
37	12.911	945	947	951	rVV4	54234	123092	2.31%	0.277%
38	13.025	955	957	958	rVV	53513	72720	1.36%	0.163%
39	13.082	960	962	964	rVV	97156	96764	1.81%	0.217%
40	13.128	964	966	969	rVB2	45844	81950	1.54%	0.184%
41	13.425	989	992	995	rBV2	127627	157659	2.95%	0.354%
42	13.631	1007	1010	1012	rBV3	45823	98877	1.85%	0.222%
43	13.745	1018	1020	1023	rVB2	204095	282973	5.30%	0.636%
44	13.882	1029	1032	1039	rBV2	837392	1371324	25.69%	3.081%
45	14.065	1046	1048	1050	rBV	152468	140181	2.63%	0.315%
46	14.271	1064	1066	1068	rBV	43558	59197	1.11%	0.133%
47	14.374	1073	1075	1076	rBV	115255	134675	2.52%	0.303%
48	14.648	1096	1099	1103	rBV3	103822	253195	4.74%	0.569%
49	14.888	1118	1120	1124	rBV	133233	250545	4.69%	0.563%
50	15.162	1142	1144	1147	rVV	68102	89730	1.68%	0.202%
51	15.220	1147	1149	1152	rVV	91836	136076	2.55%	0.306%
52	15.277	1152	1154	1161	rVB	554582	760041	14.24%	1.708%

Sum of corrected areas: 44508598

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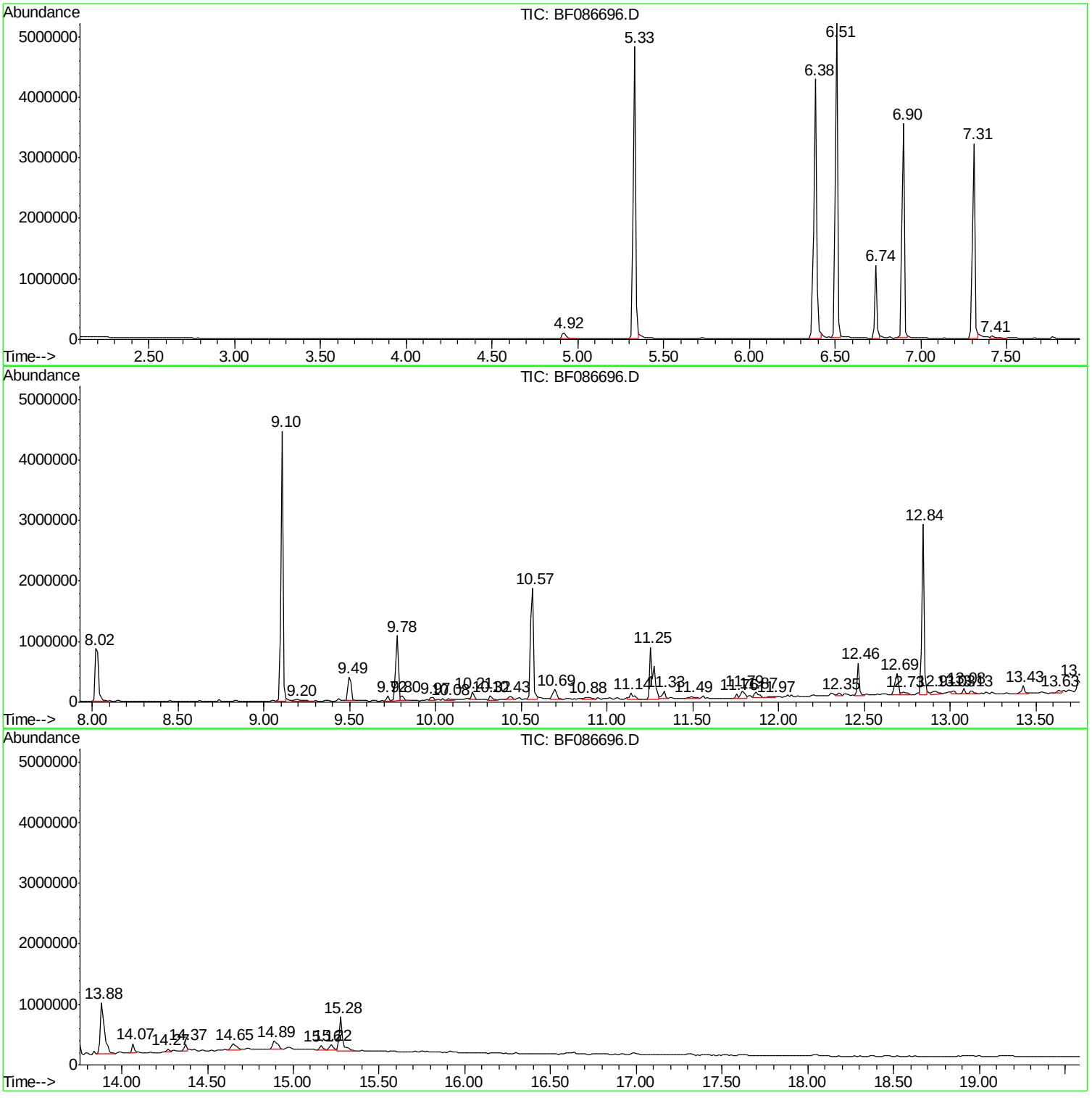
BNA_F
ClientSampleId :
26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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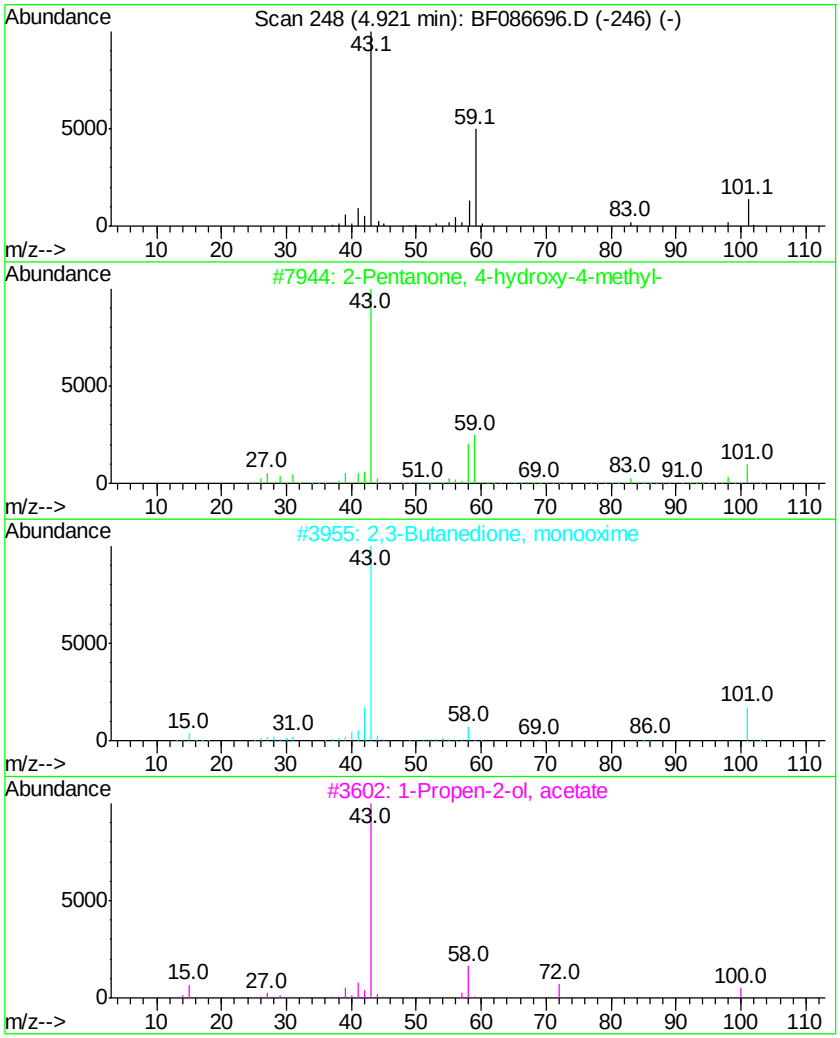
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

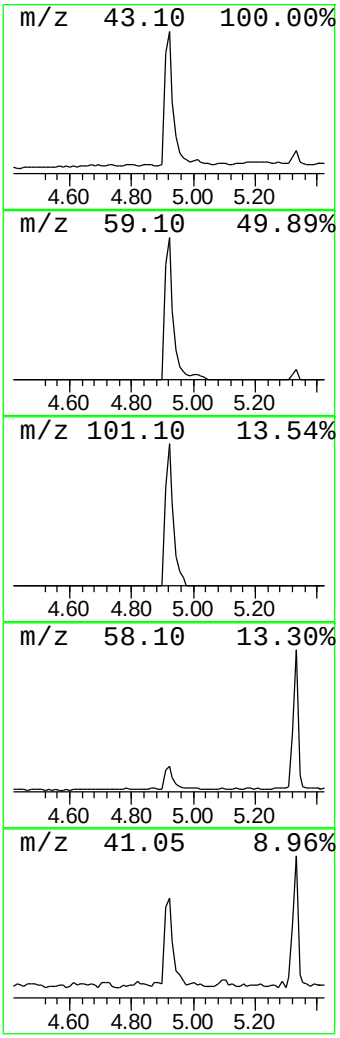
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	6.90 ng	184200	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Butane	58	C4H10	000106-97-8	9





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Sample : H2715-14
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Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
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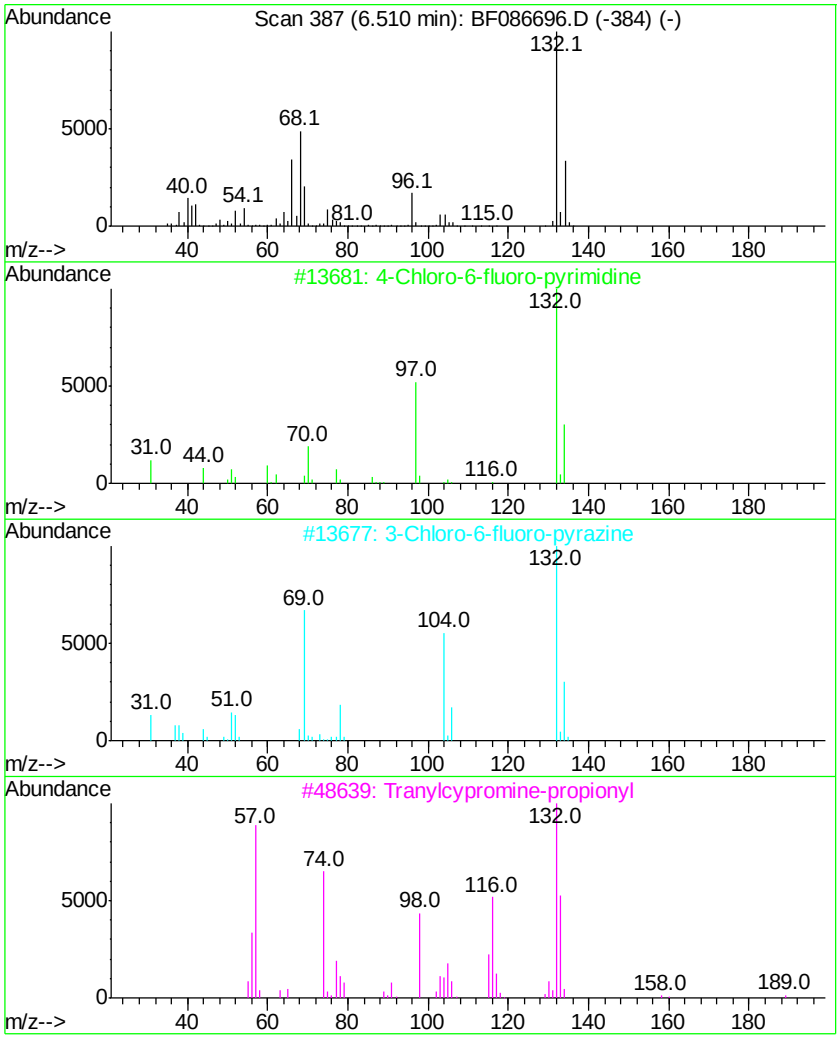
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

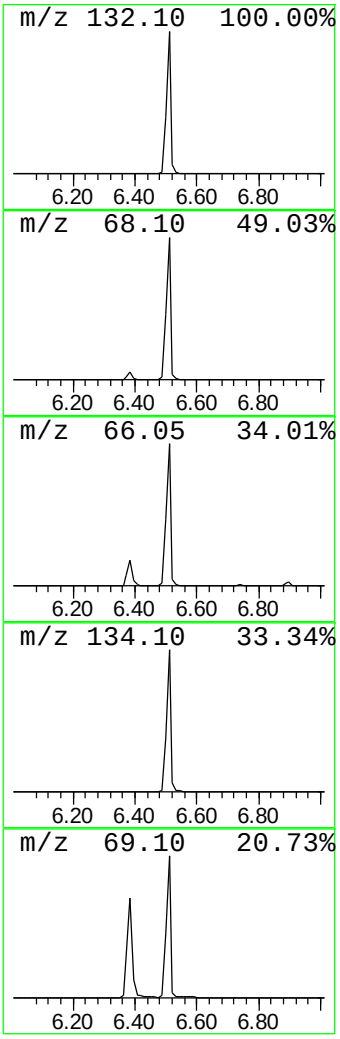
****

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	199.85 ng	5337130	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	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	16





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Operator : UM/SJ
Sample : H2715-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
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TIC Library : C:\DATABASE\NIST02.L
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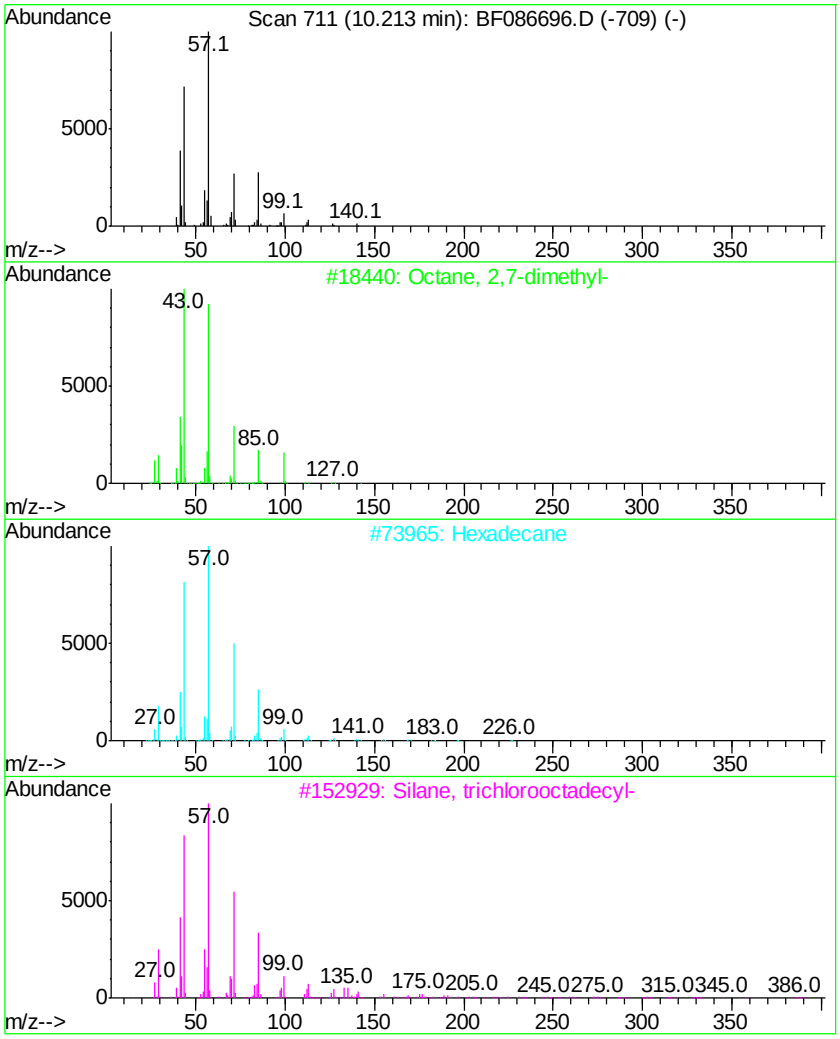
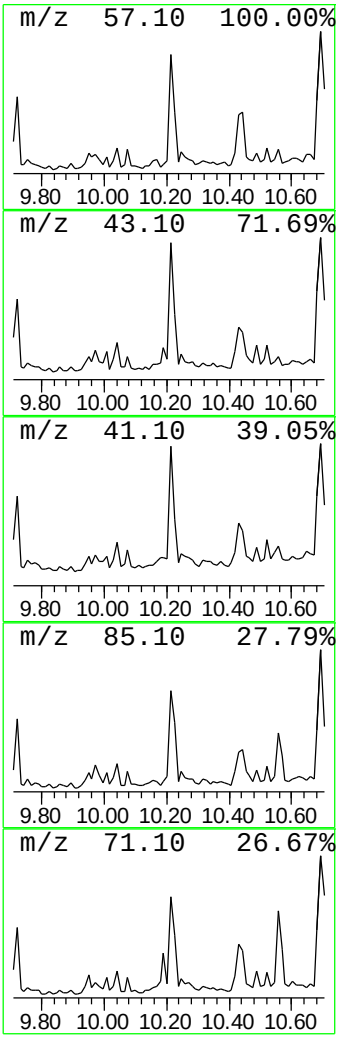
****

Peak Number 4 Octane, 2,7-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.21	4.80 ng	136121	Acenaphthene-d10	9.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	64
2	Hexadecane	226	C16H34	000544-76-3	64
3	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	53
4	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	50
5	Tetradecane	198	C14H30	000629-59-4	50





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Sample : H2715-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
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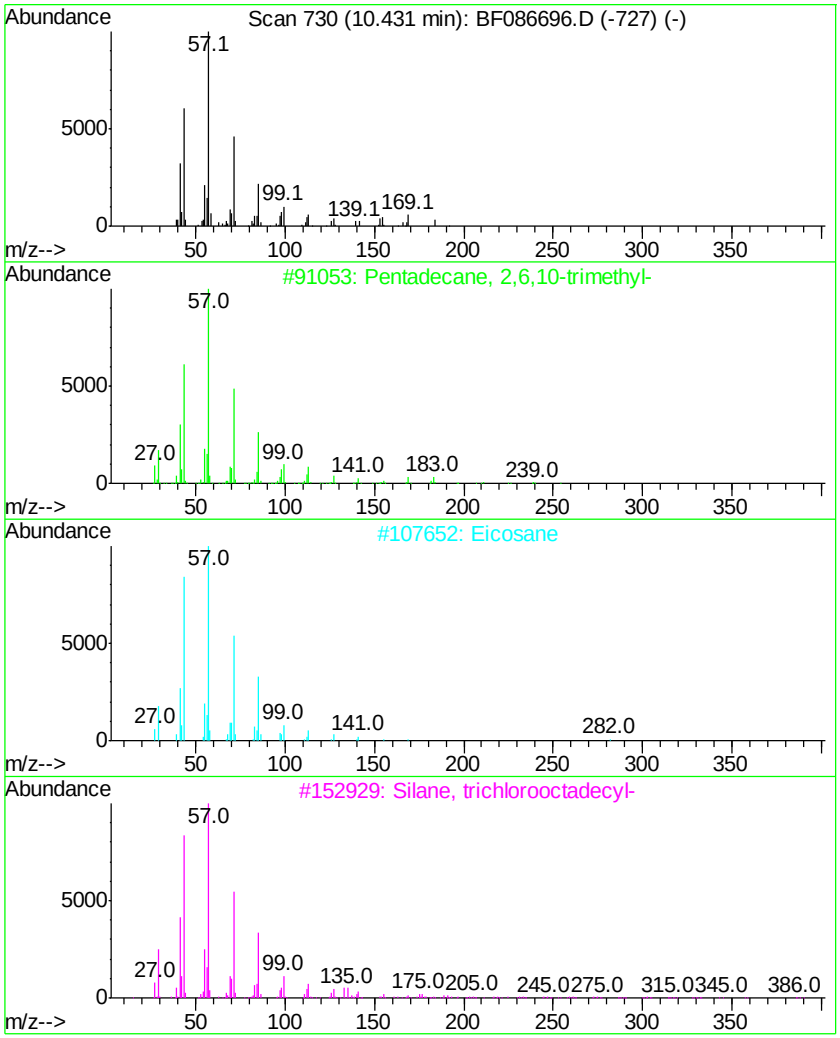
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

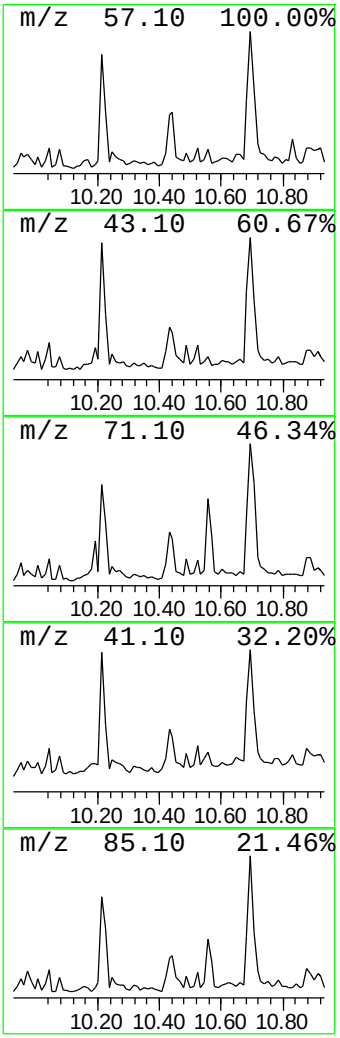
****

Peak Number 5 Pentadecane, 2,6,10-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	4.08 ng	115826	Acenaphthene-d10	9.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	80
2	Eicosane	282	C20H42	000112-95-8	64
3	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	64
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
5	Hexadecane	226	C16H34	000544-76-3	59





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Misc :
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Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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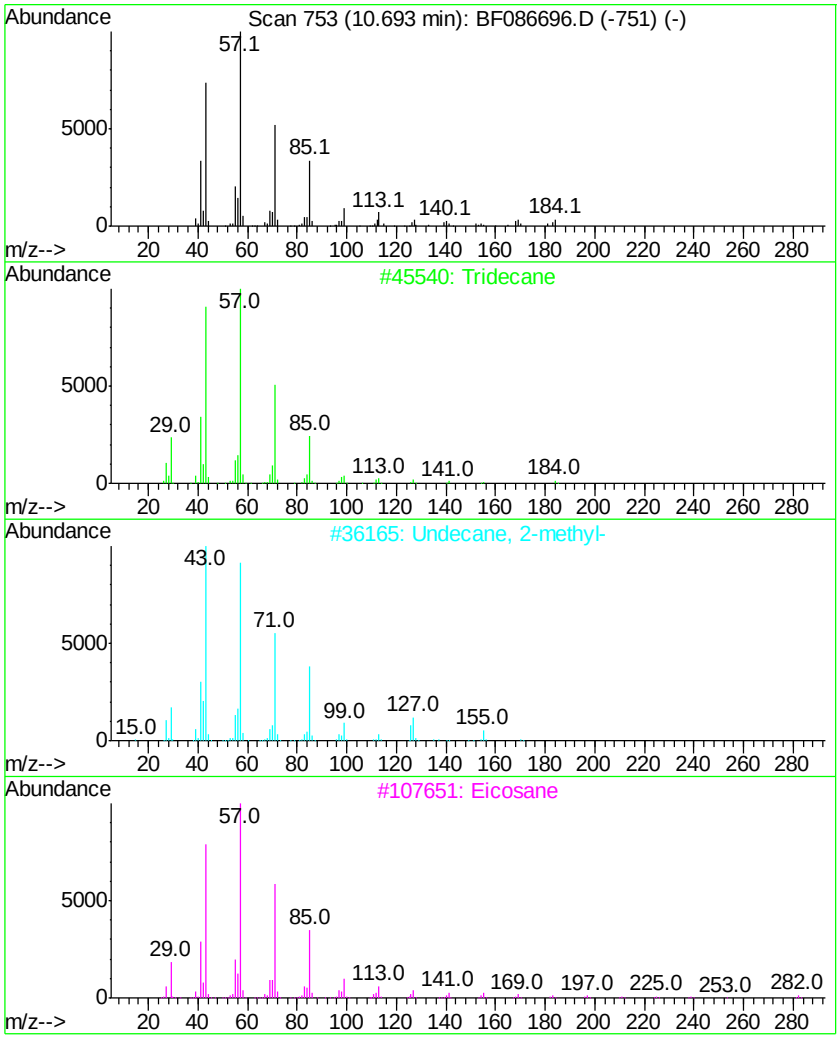
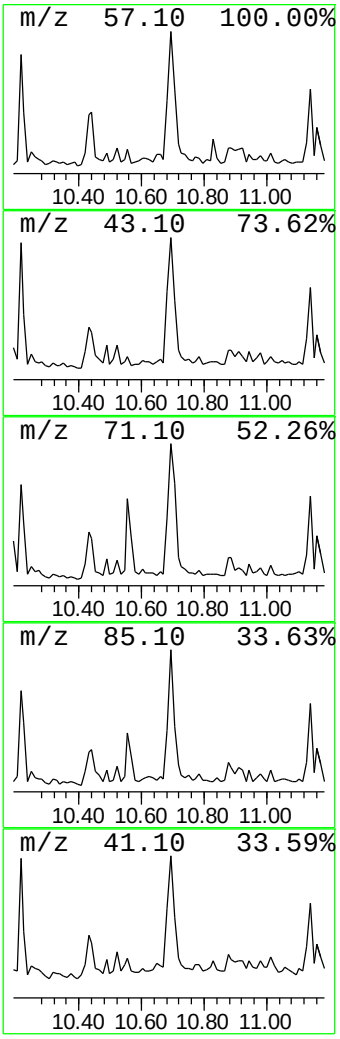
Peak Number 6 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	6.57 ng	226647	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Undecane, 2-methyl-	170	C12H26	007045-71-8	86
3	Eicosane	282	C20H42	000112-95-8	86
4	Tridecane, 2-methyl-	198	C14H30	001560-96-9	86
5	Hexadecane	226	C16H34	000544-76-3	86





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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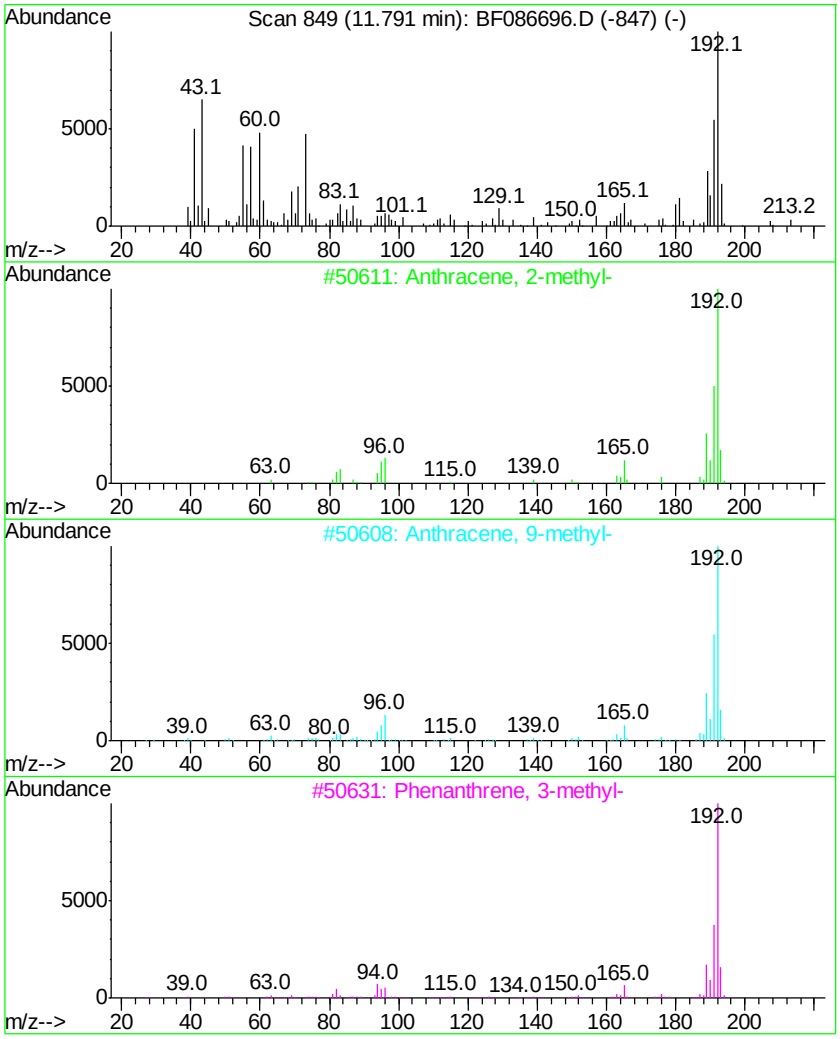
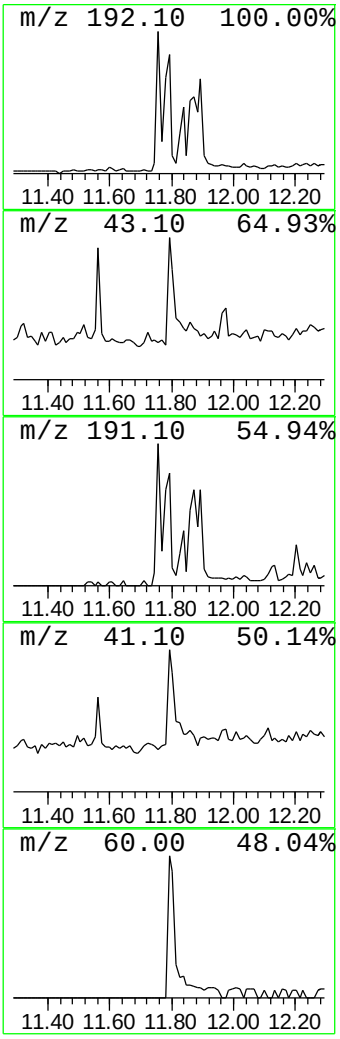
Peak Number 8 Anthracene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	5.56 ng	191701	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	78
3	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	60
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	60
5	Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	60





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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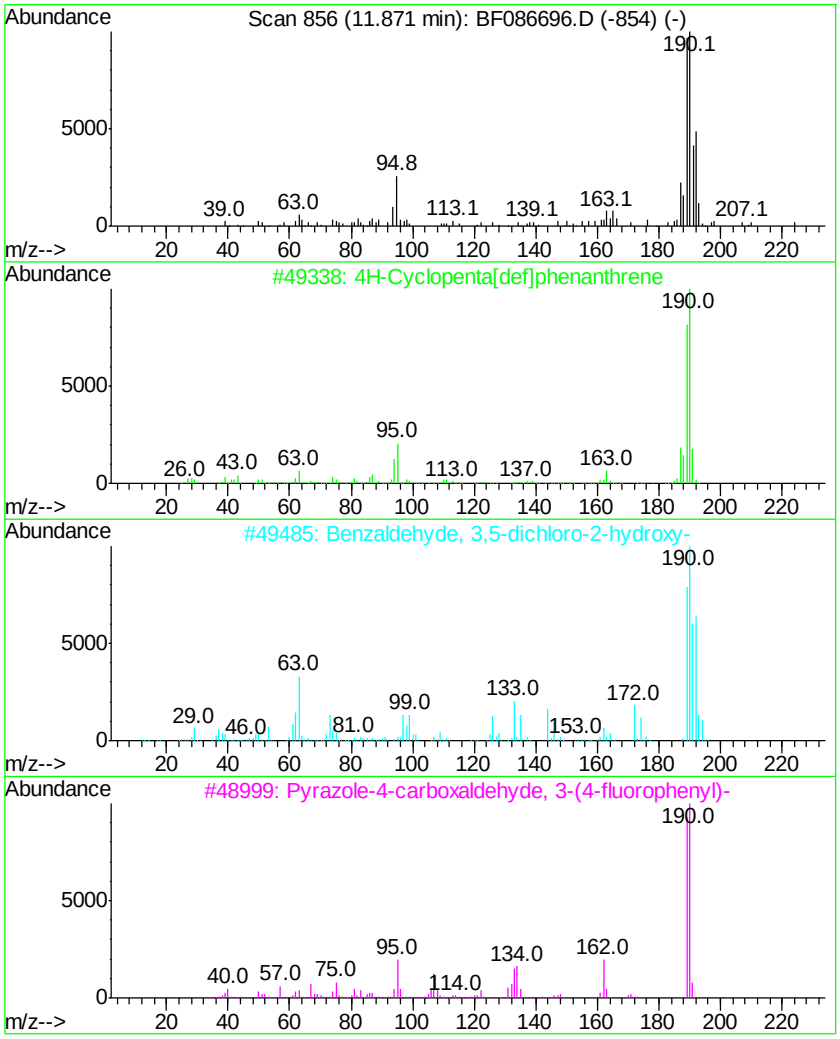
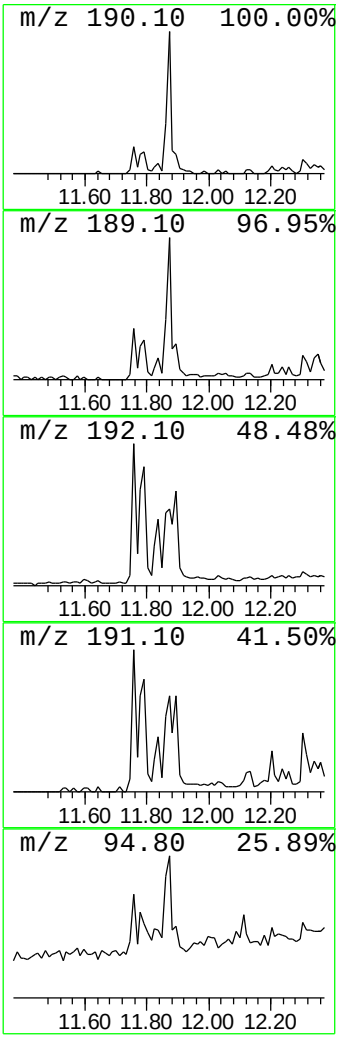
Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	5.01 ng	172756	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
4	1-(2,3-Dichloro-4-hydroxy-phenyl...	246	C11H12Cl2O2	055507-79-4	17
5	2,2'-Difluorobiphenyl	190	C12H8F2	000388-82-9	17





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Operator : UM/SJ
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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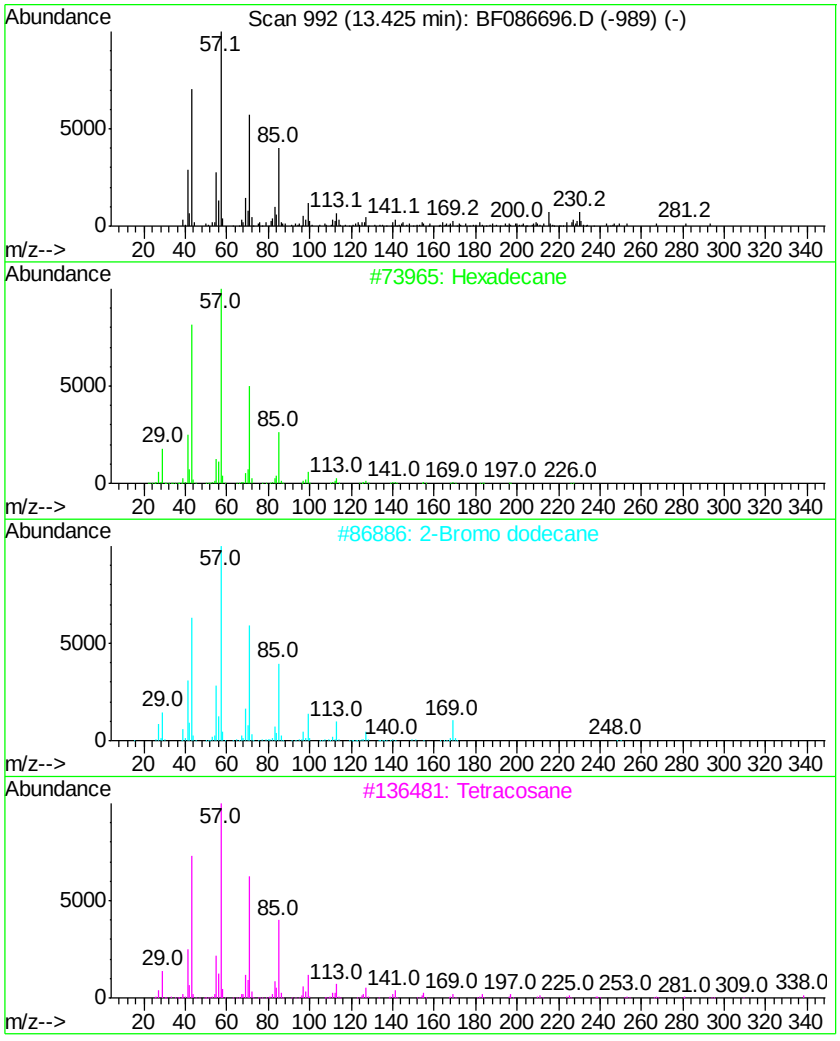
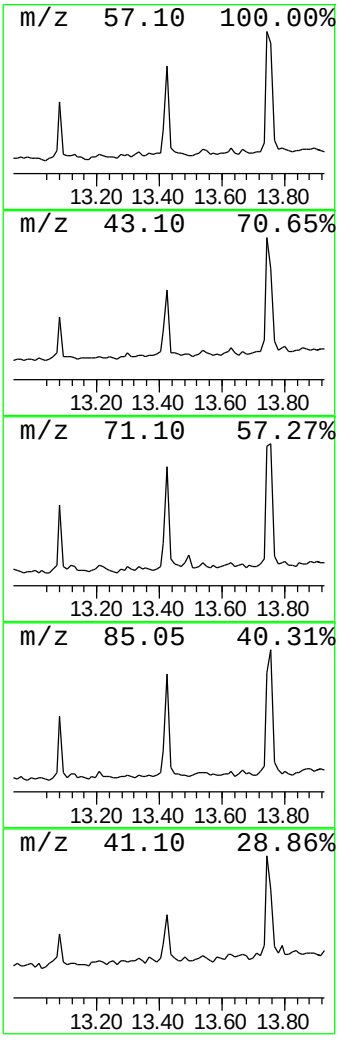
Peak Number 10 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	4.60 ng	157659	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	95
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3	Tetracosane	338	C24H50	000646-31-1	83
4	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	83
5	Octacosane	394	C28H58	000630-02-4	83





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Acq On : 5 May 2016 00:28
Operator : UM/SJ
Sample : H2715-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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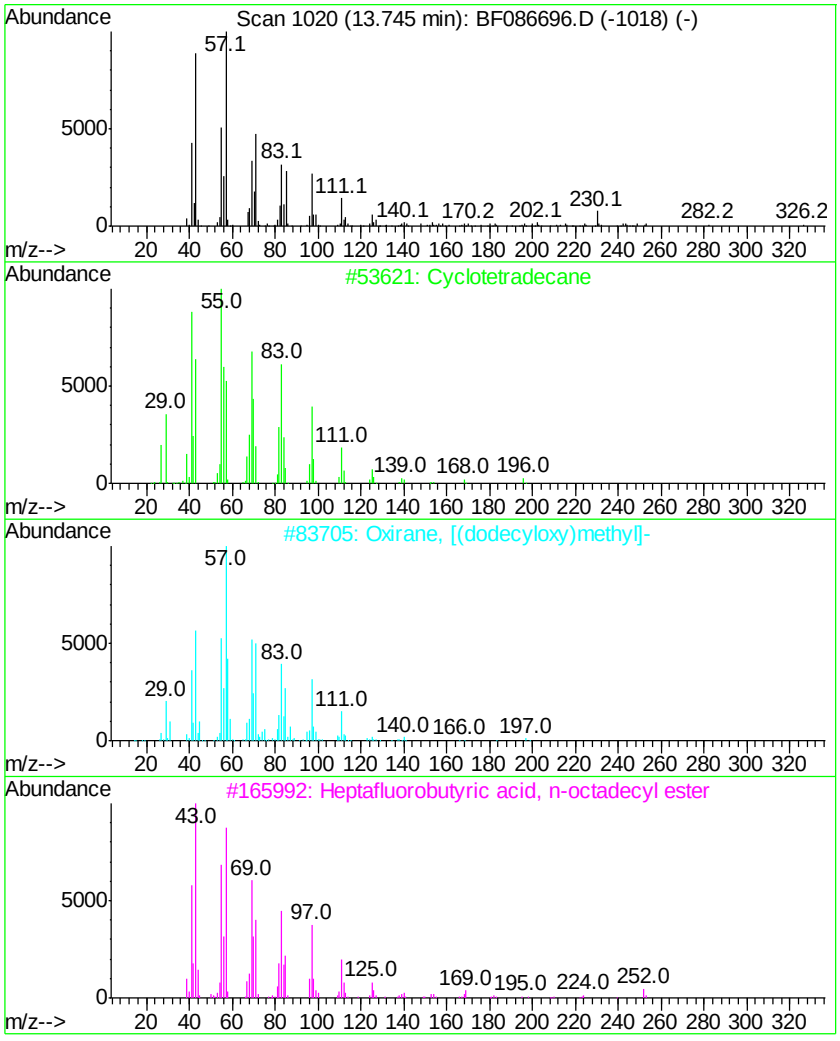
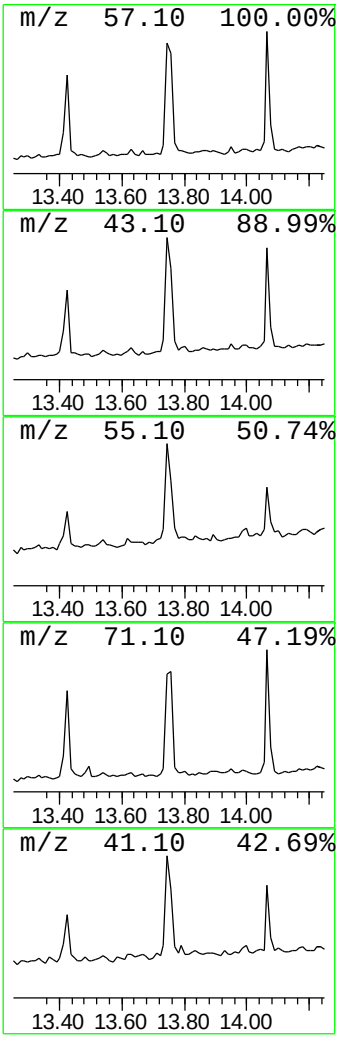
Peak Number 11 Cyclotetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	8.25 ng	282973	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	86
2	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	74
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	58
4	1-Octadecene	252	C18H36	000112-88-9	55
5	Eicosane	282	C20H42	000112-95-8	53





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Data File : BF086696.D
Acq On : 5 May 2016 00:28
Operator : UM/SJ
Sample : H2715-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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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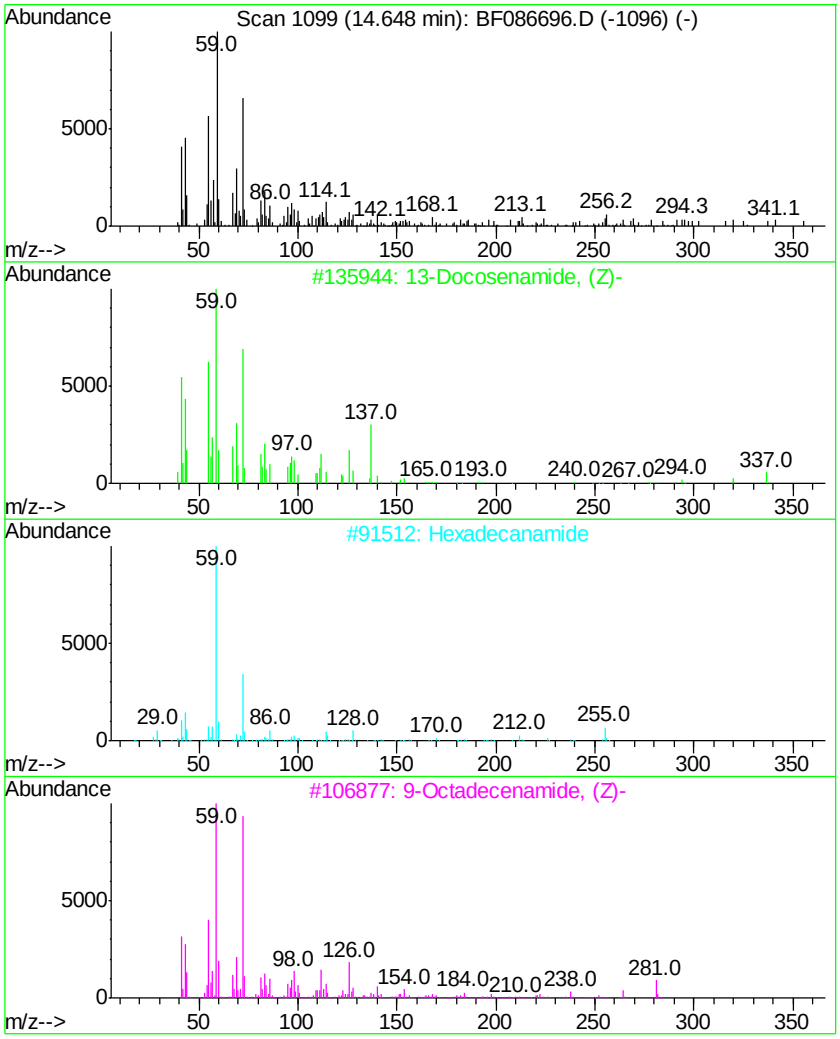
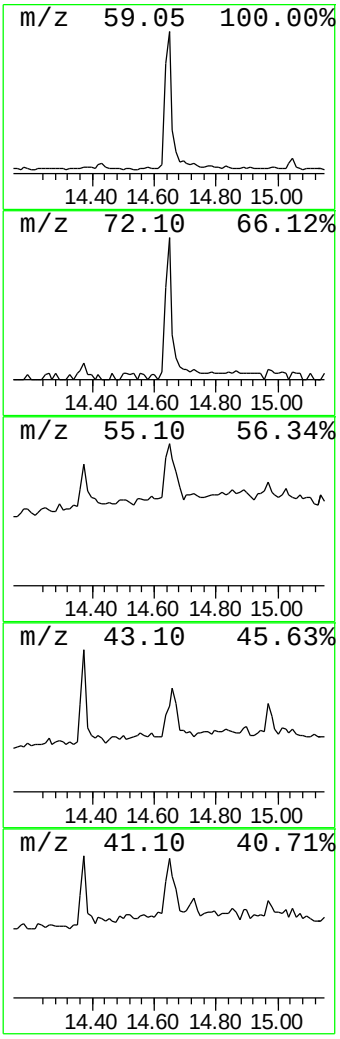
Peak Number 13 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	13.33 ng	253195	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2	Hexadecanamide	255	C16H33NO	000629-54-9	80
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	53
5	Decanamide-	171	C10H21NO	002319-29-1	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050416\
Data File : BF086696.D
Acq On : 5 May 2016 00:28
Operator : UM/SJ
Sample : H2715-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-4-CS-3(16-23FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.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...	4.92	6.9	ng	184200	1	6.74	1068250	40.0
unknown6.51	6.51	199.8	ng	5337130	1	6.74	1068250	40.0
Octane, 2,7-dimet...	10.21	4.8	ng	136121	3	9.78	1135170	40.0
Pentadecane, 2,6,...	10.43	4.1	ng	115826	3	9.78	1135170	40.0
Tridecane	10.69	6.6	ng	226647	4	11.25	1378860	40.0
Anthracene, 2-met...	11.79	5.6	ng	191701	4	11.25	1378860	40.0
4H-Cyclopenta[def...	11.87	5.0	ng	172756	4	11.25	1378860	40.0
Hexadecane	13.43	4.6	ng	157659	5	13.88	1371320	40.0
Cyclotetradecane	13.75	8.3	ng	282973	5	13.88	1371320	40.0
13-Docosenamide, ...	14.65	13.3	ng	253195	6	15.28	760041	40.0