LSC Area Percent Report

Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085344.D
Acq On : 10 Mar 2016 20:28
Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

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-BF030316.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	5.133	246	249	260	rVB	204050	252607	7.59%	0.782%
2	5.533	282	284	287	rBV	2155442	3136805	94.27%	9.714%
3	6.562	371	374	377	rBV	2542603	2751445	82.69%	8.520%
4	6.710	384	387	389	rBV	2806622	3327337	100.00%	10.304%
5	6.939	405	407	409	rBV	1071861	862774	25.93%	2.672%
6	7.099	418	421	423	rBV	2741095	2602341	78.21%	8.059%
7	7.499	453	456	458	rBV	1856413	1826419	54.89%	5.656%
8	8.219	517	519	522	rBV	964017	1077128	32.37%	3.336%
9	9.305	611	614	616	rBV	2758331	3164275	95.10%	9.799%
10	9.385	619	621	623	rBV	22504	35149	1.06%	0.109%
11	9.636	638	643	646	rBV2	26474	42447	1.28%	0.131%
12	9.693	646	648	650	rBV	352392	336312	10.11%	1.041%
13	9.910	663	667	669	rVV	112092	105531	3.17%	0.327%
14	9.979	670	673	675	rVV	1076075	937209	28.17%	2.902%
15	10.013	675	676	678	rVB	54632	38663	1.16%	0.120%
16	10.139	684	687	689	rBV2	27417	45995	1.38%	0.142%
17	10.173	689	690	693	rVV2	27587	50352	1.51%	0.156%
18	10.230	693	695	697	rVB3	32781	37377	1.12%	0.116%
19	10.413	707	711	712	rBV	99576	142376	4.28%	0.441%
20	10.528	719	721	723	rVB	38075	50626	1.52%	0.157%
21	10.630	726	730	733	rVV	50848	86625	2.60%	0.268%
22	10.768	739	742	744	rBV	1542175	1505912	45.26%	4.663%
23	10.882	749	752	756	rVV	144949	198305	5.96%	0.614%
24	11.076	766	769	770	rBV2	28161	42861	1.29%	0.133%
25	11.328	789	791	792	rVV	85136	76883	2.31%	0.238%
26	11.362	792	794	797	rVB	58662	70155	2.11%	0.217%
27	11.465	800	803	804	rBV	864043	836231	25.13%	2.590%
28	11.533	807	809	811	rVB	109348	115618	3.47%	0.358%
29	11.693	820	823	826	rBV	40196	79322	2.38%	0.246%
30	11.751	826	828	830	rVB	29722	37350	1.12%	0.116%
31	11.991	844	849	851	rBV	108413	180441	5.42%	0.559%
32	12.071	854	856	861	rVB	84260	162858	4.89%	0.504%
33	12.254	870	872	876	rVB3	29076	61403	1.85%	0.190%
34	12.414	882	886	887	rBV2	26460	49973	1.50%	0.155%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.516	892	895	896	rBV	49030	58372	1.75%	0.181%
36	12.551	896	898	901	rVV2	46464	57476	1.73%	0.178%
37	12.676	906	909	911	rBV	589427	537037	16.14%	1.663%
38	12.768	915	917	921	rBV3	52779	89512	2.69%	0.277%
39	12.905	926	929	931	rBV	554287	610793	18.36%	1.891%
40	12.951	932	933	936	rBV2	24517	36157	1.09%	0.112%
41	13.054	939	942	944	rVV	1810670	2196811	66.02%	6.803%
42	13.122	945	948	952	rBV3	43506	108014	3.25%	0.334%
43	13.236	955	958	959	rVB	54452	91829	2.76%	0.284%
44	13.294	961	963	965	rVV2	48717	71026	2.13%	0.220%
45	13.339	965	967	970	rVB4	49296	86864	2.61%	0.269%
46	13.945	1018	1020	1025	rVB2	130922	172644	5.19%	0.535%
47	14.105	1030	1034	1039	rVB2	654445	1256359	37.76%	3.891%
48	14.859	1098	1100	1103	rBV	271739	321448	9.66%	0.995%
49	15.145	1122	1125	1129	rBV	206151	473315	14.23%	1.466%
50	15.442	1148	1151	1154	rBV	133840	191237	5.75%	0.592%
51	15.500	1154	1156	1160	rVV	202948	290772	8.74%	0.900%
52	15.568	1160	1162	1168	rVB	533776	808457	24.30%	2.504%
53	16.277	1222	1224	1231	rVB	89073	184956	5.56%	0.573%
54	17.020	1286	1289	1295	rVB2	88757	177760	5.34%	0.550%
55	17.454	1325	1327	1335	rVB	57205	144193	4.33%	0.447%

Sum of corrected areas: 32292137

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Acq On : 10 Mar 2016 20:28
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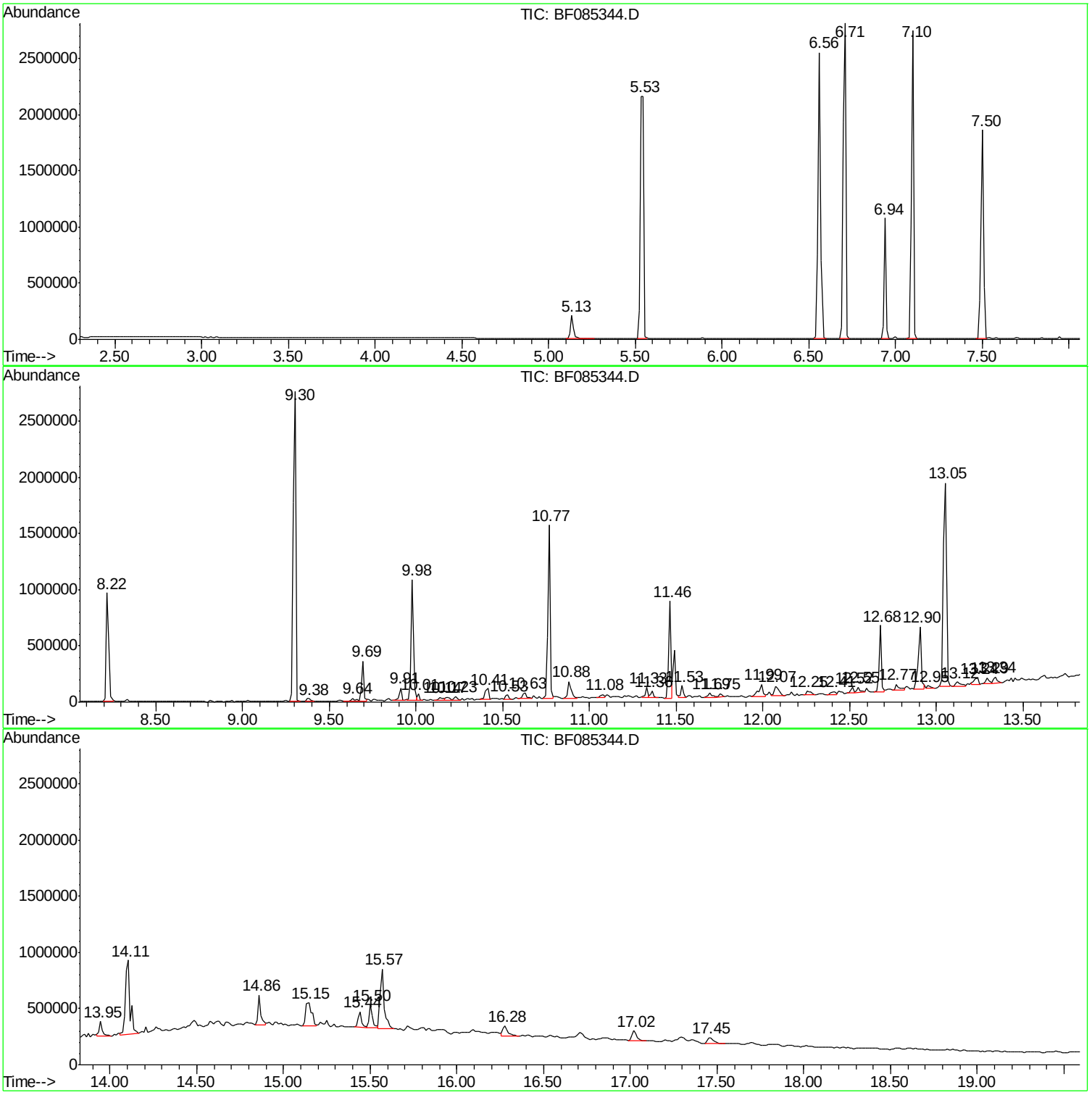
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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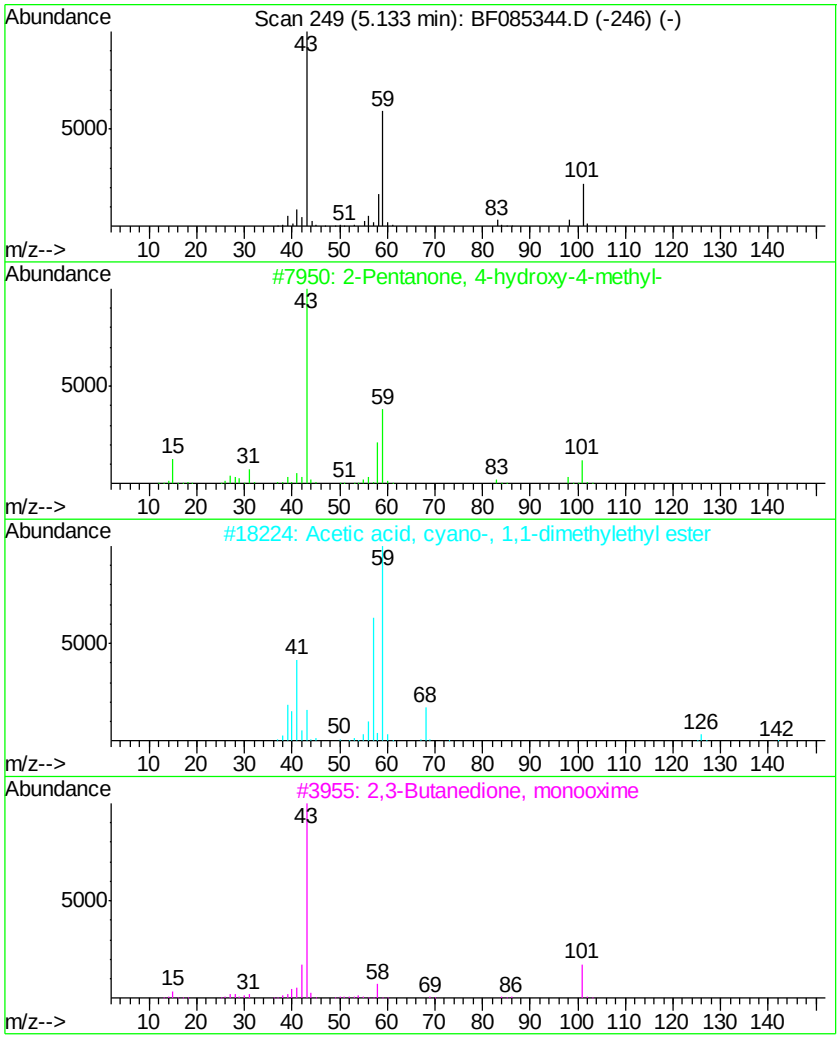
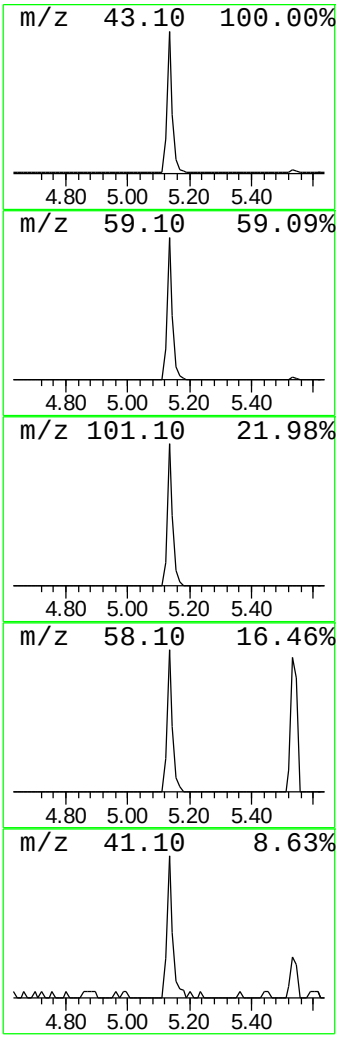
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	5.86 ng	252607	1,4-Dichlorobenzene-d4	6.94

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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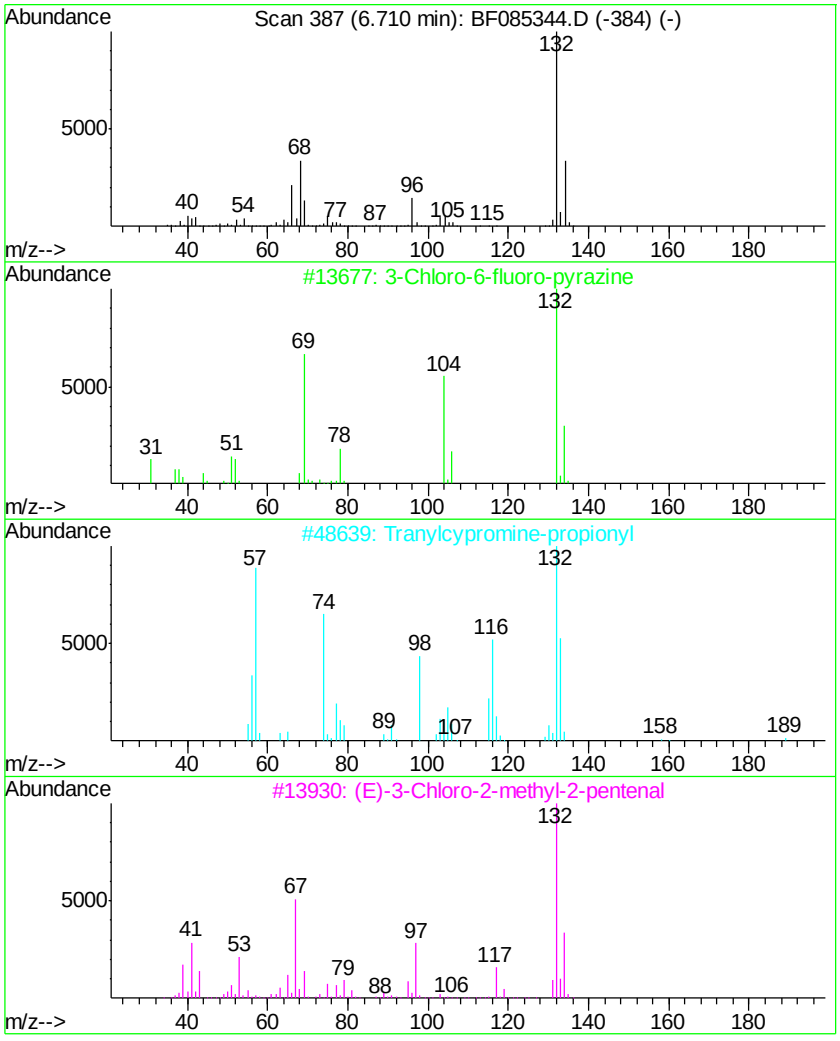
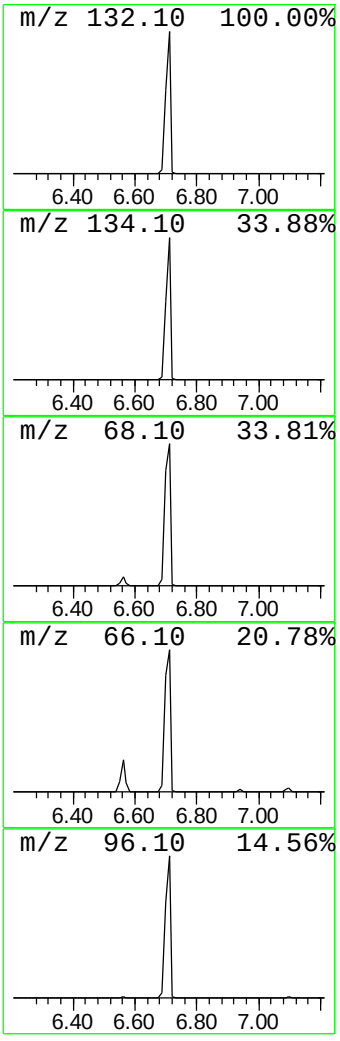
Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	77.13 ng	3327340	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Acq On : 10 Mar 2016 20:28
Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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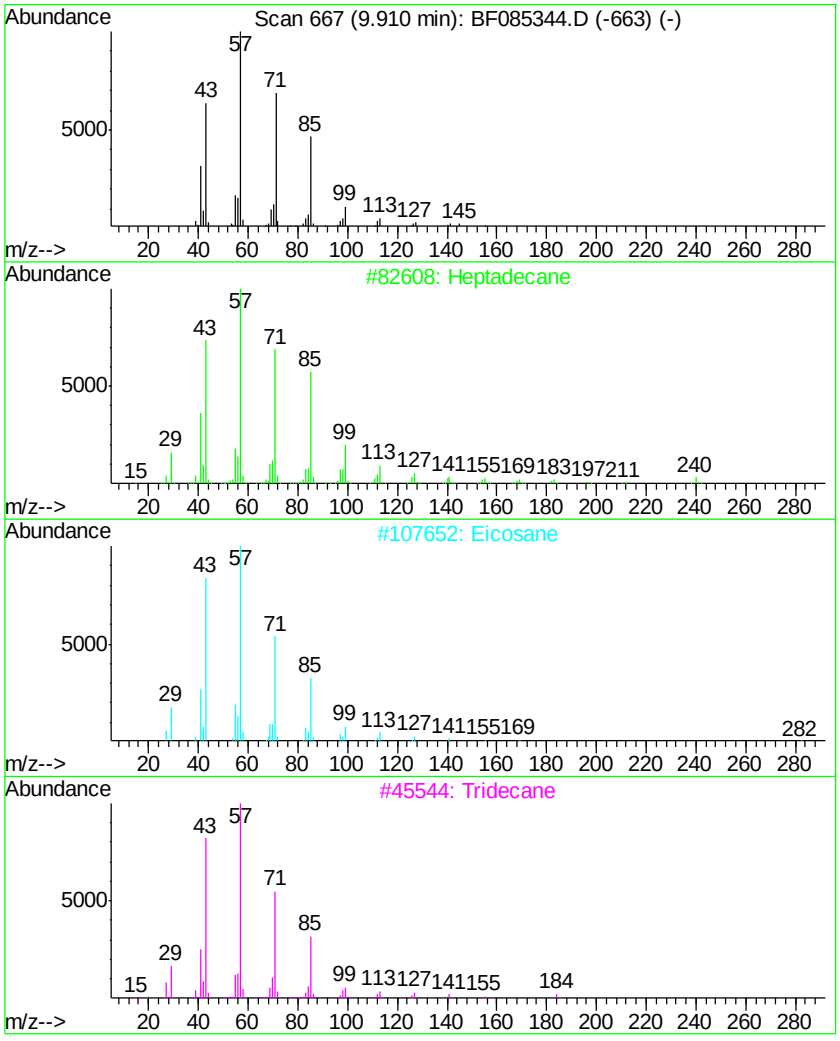
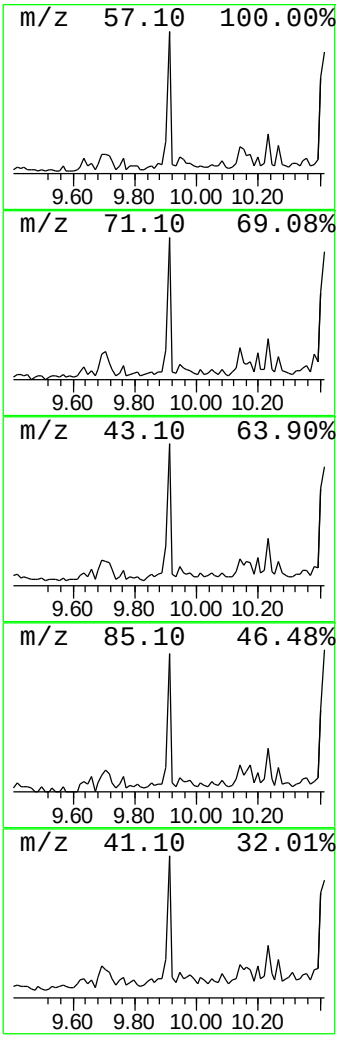
Peak Number 4 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.91	2.25 ng	105531	Acenaphthene-d10	9.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tridecane	184	C13H28	000629-50-5	90
4	Tetradecane	198	C14H30	000629-59-4	87
5	Pentadecane	212	C15H32	000629-62-9	78





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Acq On : 10 Mar 2016 20:28
Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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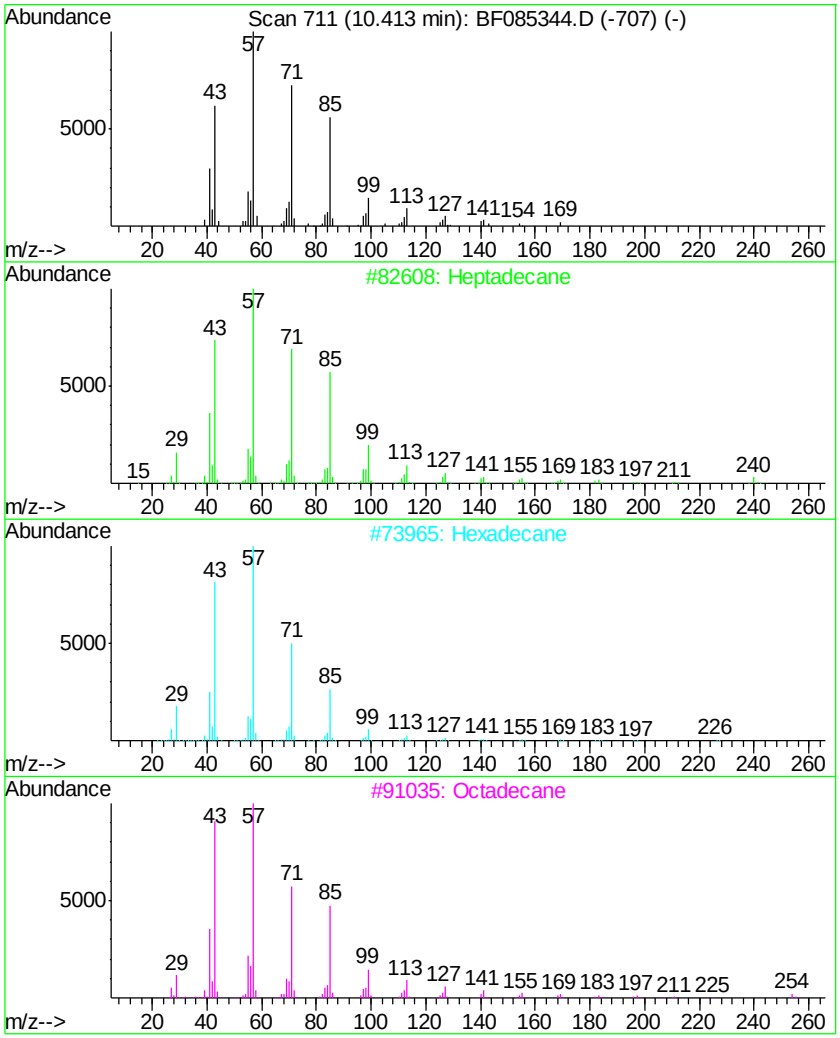
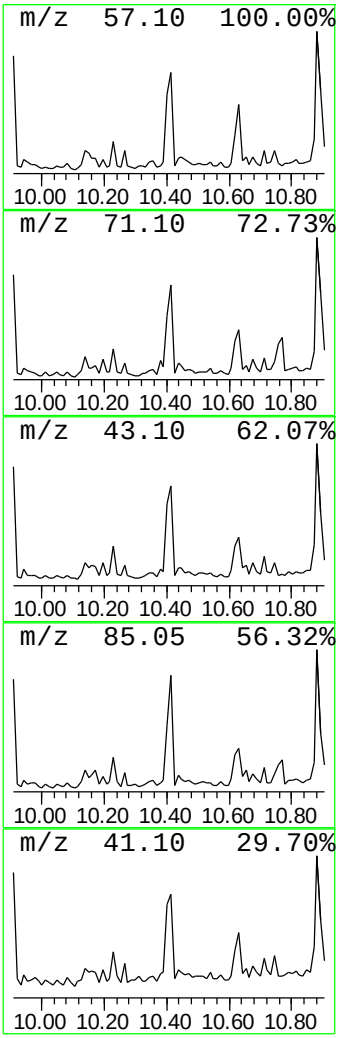
Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	3.04 ng	142376	Acenaphthene-d10	9.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Pentadecane	212	C15H32	000629-62-9	87
5	Tetradecane	198	C14H30	000629-59-4	86





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Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
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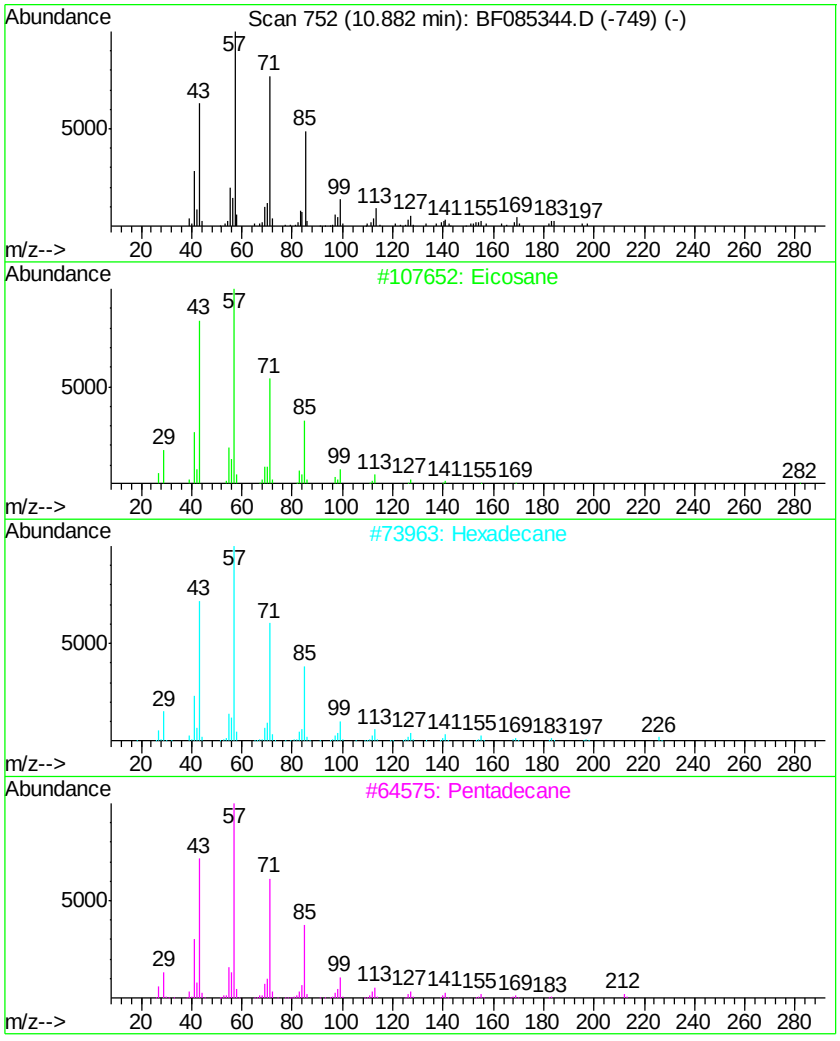
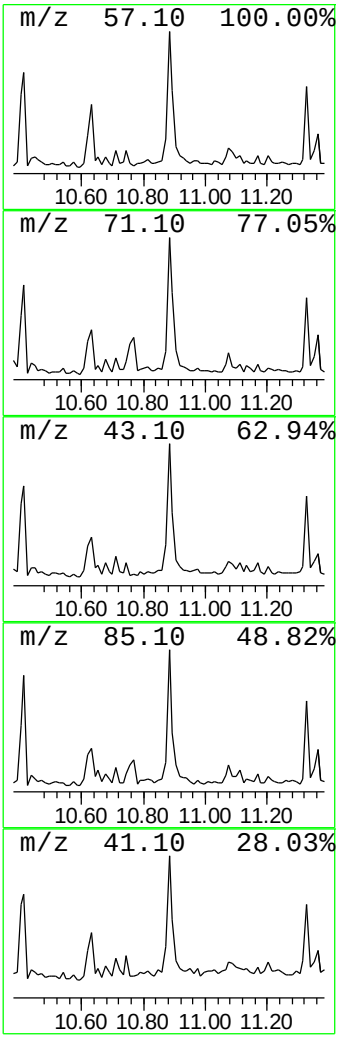
Peak Number 6 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	4.74 ng	198305	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Pentadecane	212	C15H32	000629-62-9	91
4	Dodecane	170	C12H26	000112-40-3	87
5	Tetracosane	338	C24H50	000646-31-1	87





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Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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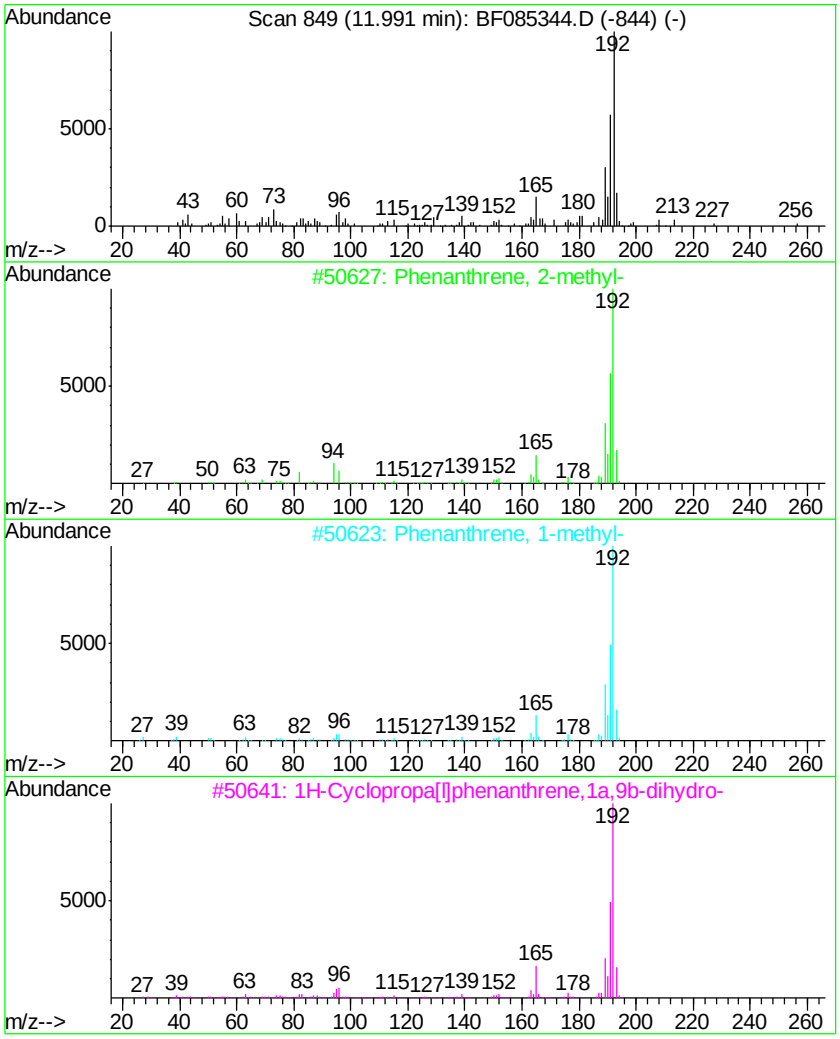
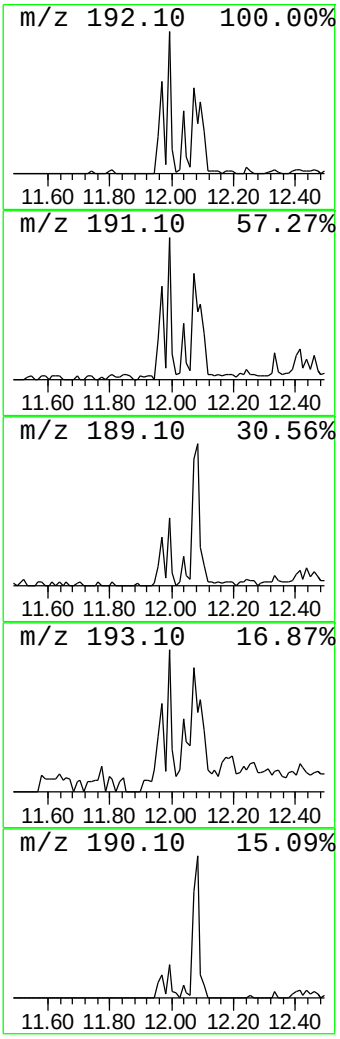
Peak Number 7 Phenanthrene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	4.32 ng	180441	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	96
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93





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Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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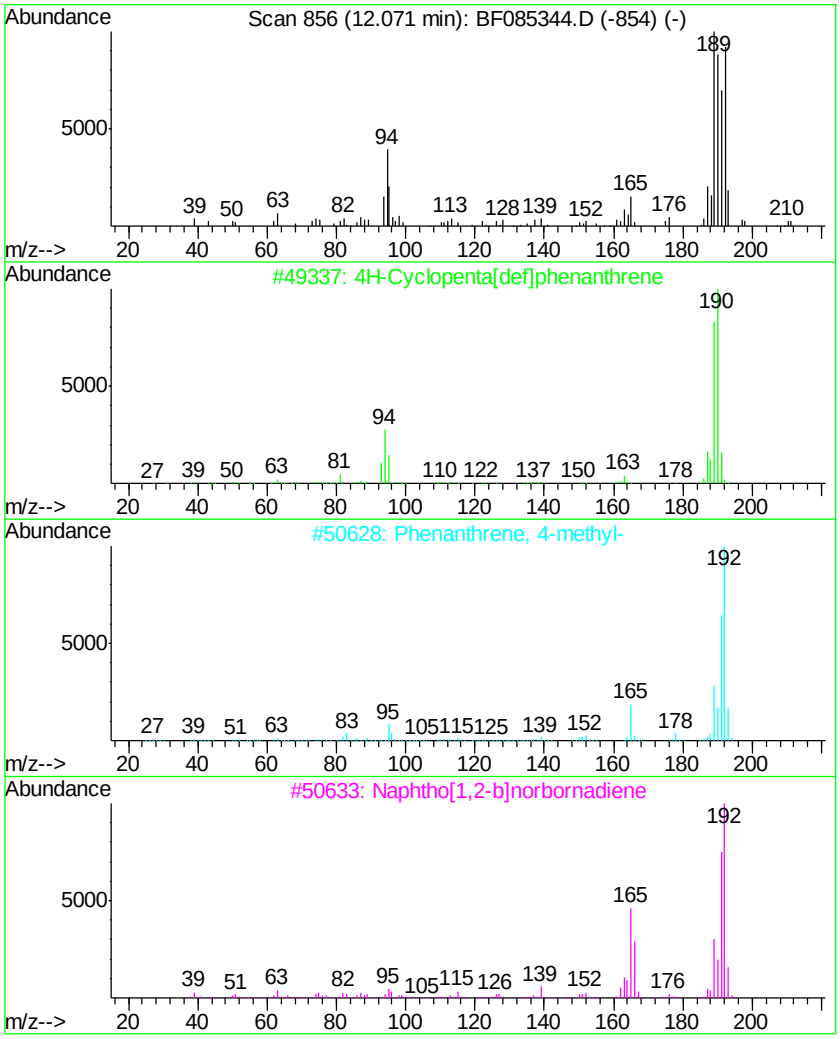
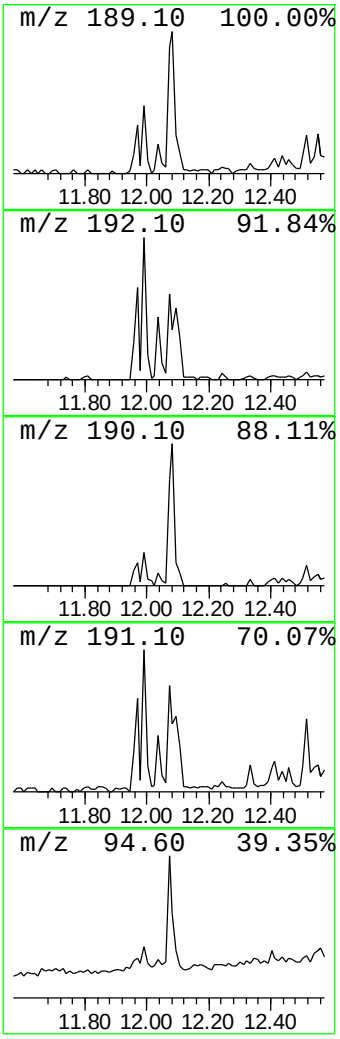
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	3.90 ng	162858	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	86
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
3	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	38
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	38
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	30





Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085344.D
Acq On : 10 Mar 2016 20:28
Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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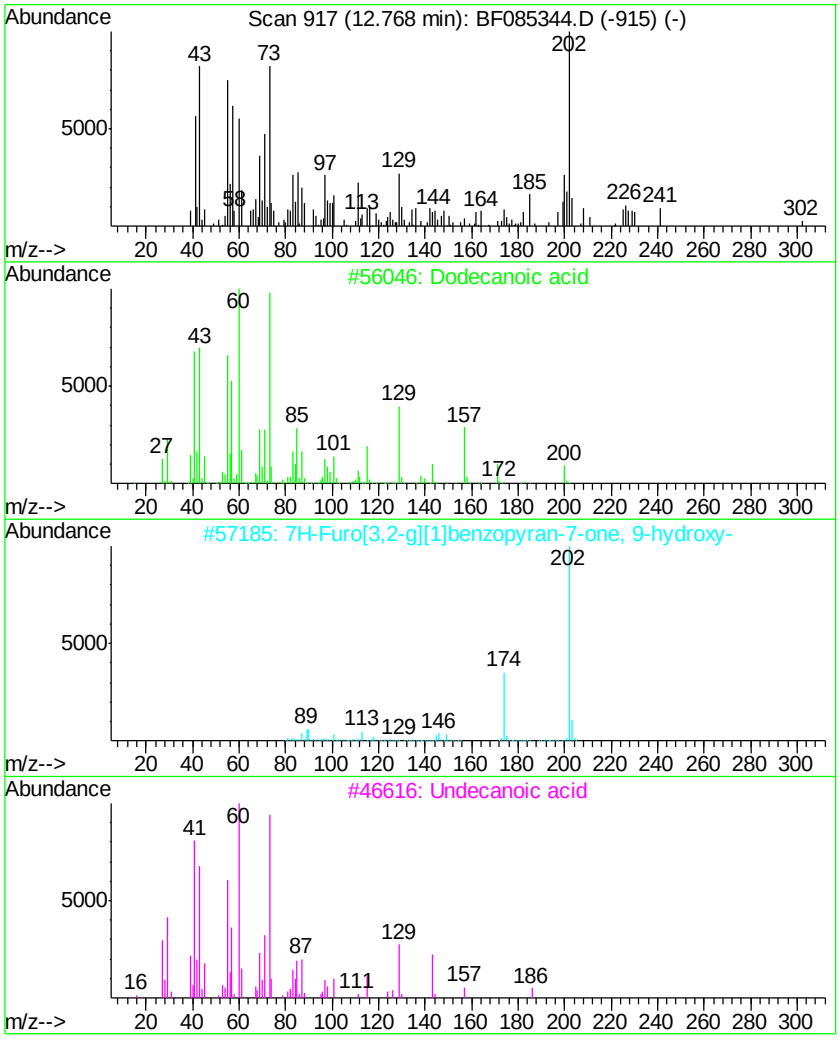
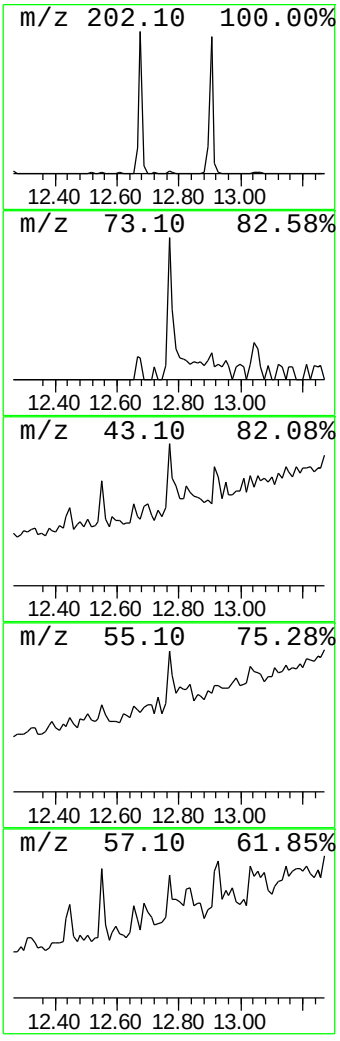
Peak Number 9 unknown12.77 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	2.14 ng	89512	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	35
2	7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	002009-24-7	27
3	Undecanoic acid	186	C11H22O2	000112-37-8	27
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	27
5	Pyrene	202	C16H10	000129-00-0	22





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Acq On : 10 Mar 2016 20:28
Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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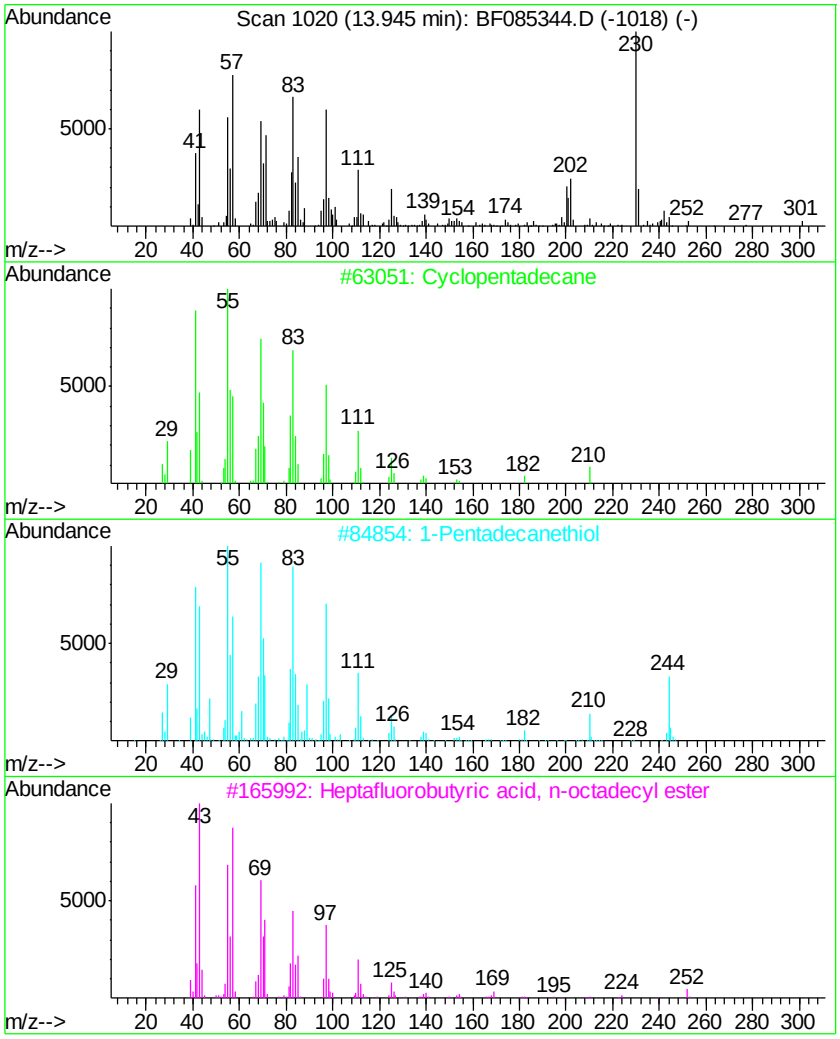
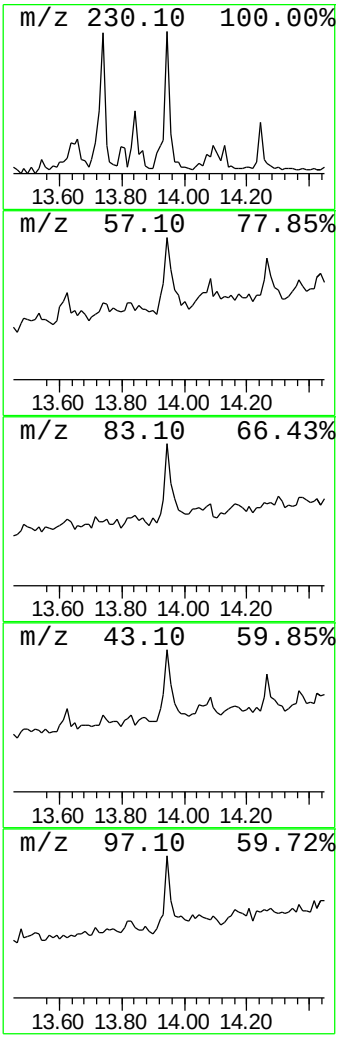
Peak Number 10 Cyclopentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.75 ng	172644	Chrysene-d12	14.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	81
2	1-Pentadecanethiol	244	C15H32S	025276-70-4	59
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	55
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	55
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	55





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Acq On : 10 Mar 2016 20:28
Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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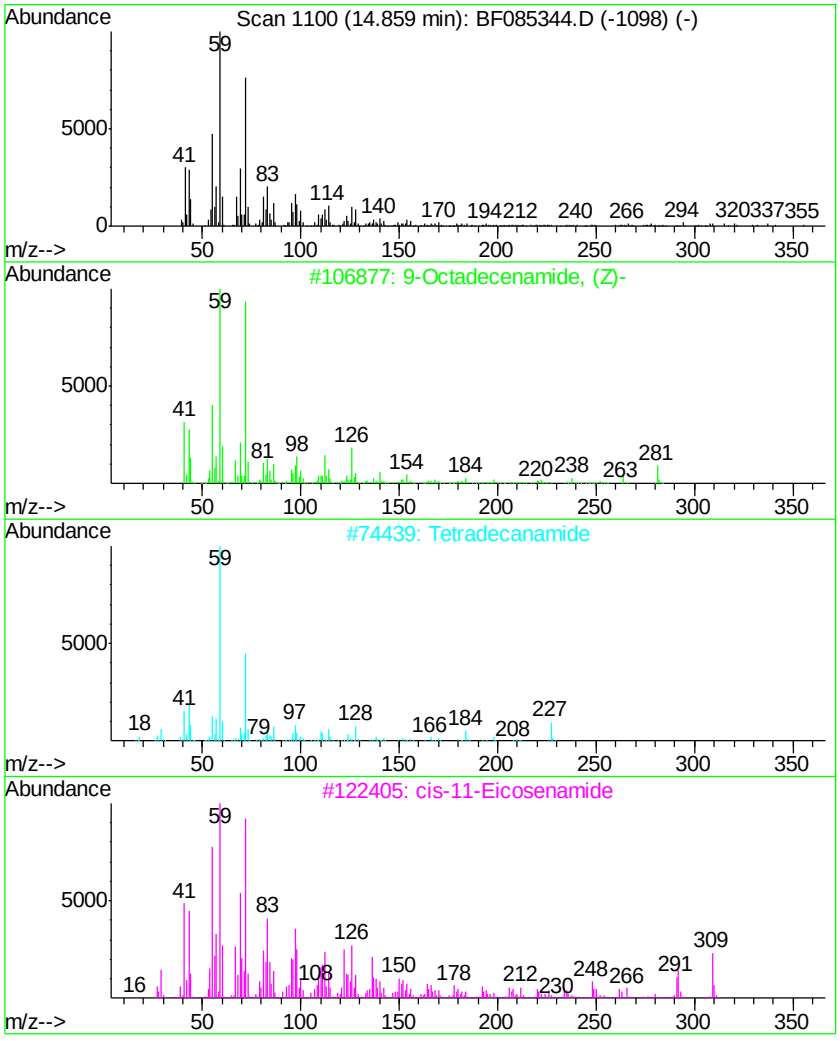
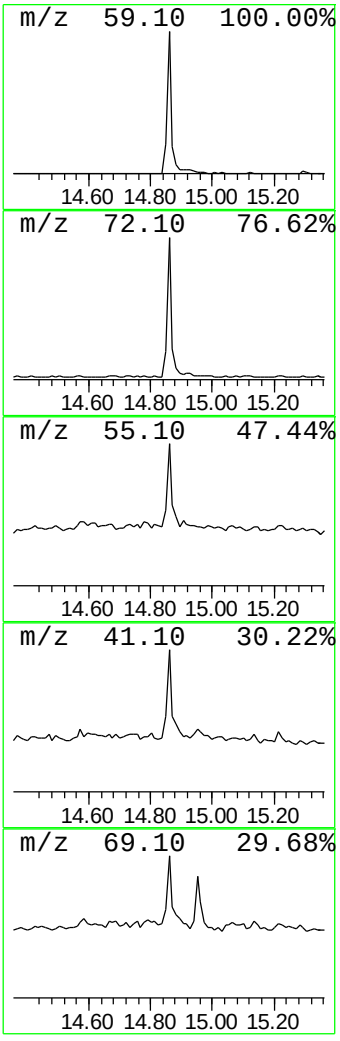
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	7.95 ng	321448	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	64
2	Tetradecanamide	227	C14H29NO	000638-58-4	50
3	cis-11-Eicosenamide	309	C20H39NO	010436-08-5	46
4	Dodecanamide	199	C12H25NO	001120-16-7	43
5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	43





Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085344.D
Acq On : 10 Mar 2016 20:28
Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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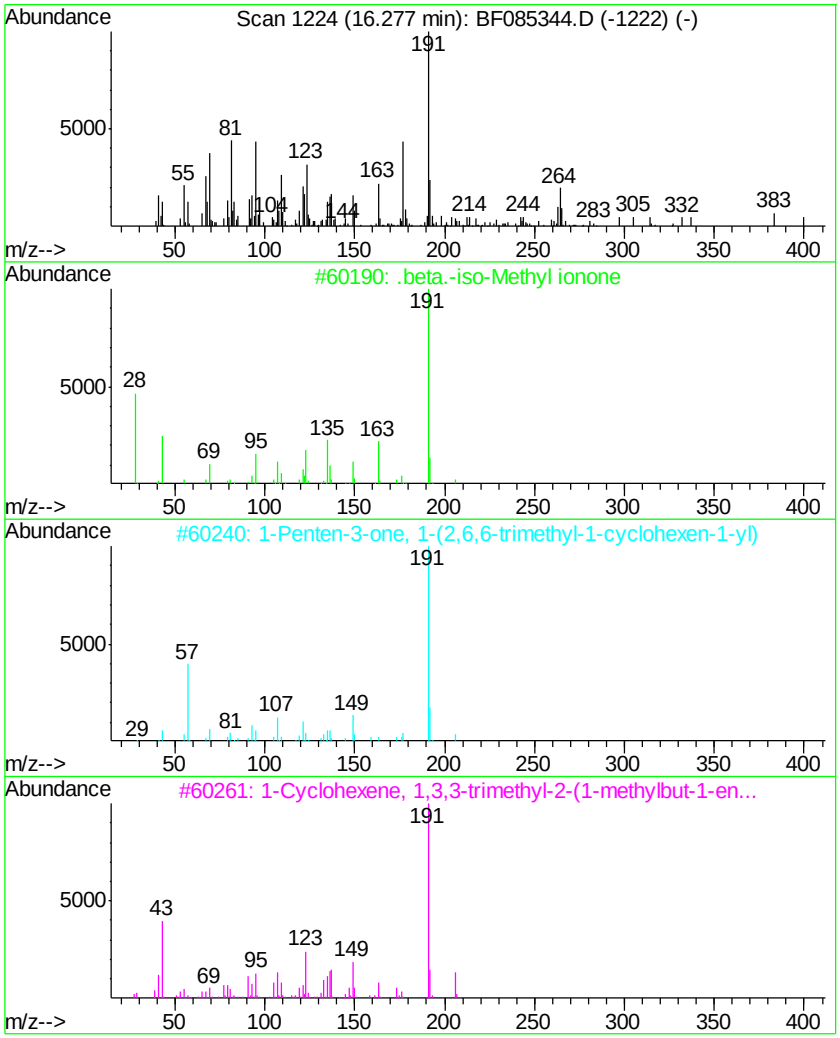
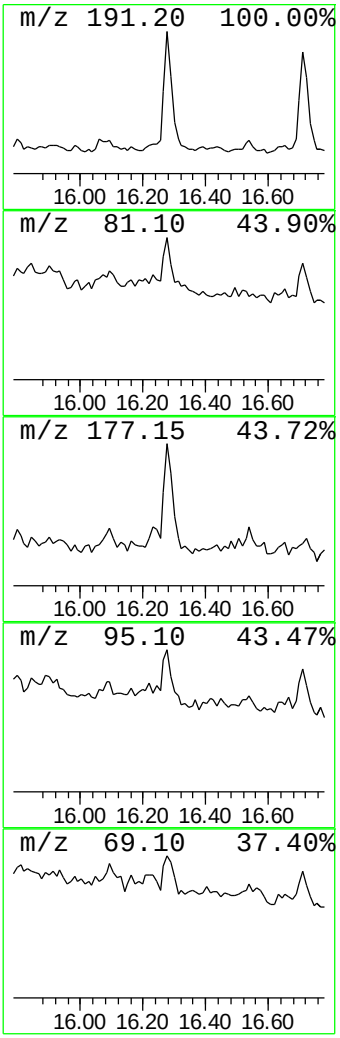
Peak Number 13 .beta.-iso-Methyl ionone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.28	4.58 ng	184956	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	52
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	30
3	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	25
4	5-(1-Isopropenyl-4,5-dimethylbic...	332	C22H36O2	1000195-69-8	25
5	2'-Fluoro-6'-(trifluoromethyl)-a...	206	C9H6F4O	174013-29-7	22





Tentatively Identified Compound (LSC) summary

Data Path : S:\HPCHEM1\BNA_F\DATA\BF031016\
Data File : BF085344.D
Acq On : 10 Mar 2016 20:28
Operator : UM/SJ
Sample : H1753-23
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-COMP5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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...	5.13	5.9	ng	252607	1	6.94	862774	20.0
unknown6.71	6.71	77.1	ng	3327340	1	6.94	862774	20.0
Heptadecane	9.91	2.3	ng	105531	3	9.98	937209	20.0
Hexadecane	10.41	3.0	ng	142376	3	9.98	937209	20.0
Eicosane	10.88	4.7	ng	198305	4	11.46	836231	20.0
Phenanthrene, 2-m...	11.99	4.3	ng	180441	4	11.46	836231	20.0
4H-Cyclopenta[def...	12.07	3.9	ng	162858	4	11.46	836231	20.0
unknown12.77	12.77	2.1	ng	89512	4	11.46	836231	20.0
Cyclopentadecane	13.95	2.8	ng	172644	5	14.11	1256360	20.0
9-Octadecenamide,...	14.86	8.0	ng	321448	6	15.57	808457	20.0
.beta.-iso-Methyl...	16.28	4.6	ng	184956	6	15.57	808457	20.0