LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086480.D
Acq On : 28 Apr 2016 23:20
Operator : UM/SJ
Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

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-BF042716.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	4.978	250	253	258	rBV	68795	114528	2.46%	0.287%
2	5.378	285	288	291	rBV	2854637	3892182	83.70%	9.738%
3	6.430	376	380	382	rBV	3750674	4650019	100.00%	11.634%
4	6.556	388	391	393	rBV	4051866	4141174	89.06%	10.361%
5	6.624	393	397	399	rVB	86905	96821	2.08%	0.242%
6	6.784	409	411	416	rBV	1087236	1013010	21.79%	2.534%
7	6.944	422	425	427	rBV	3348990	3146519	67.67%	7.872%
8	7.356	458	461	463	rBV	2647900	2895322	62.26%	7.244%
9	7.459	467	470	477	rVB	68596	160407	3.45%	0.401%
10	8.076	521	524	526	rBV	1089628	1265748	27.22%	3.167%
11	9.150	615	618	621	rBV	3650317	3777405	81.23%	9.451%
12	9.550	651	653	655	rBV	360869	434072	9.33%	1.086%
13	9.767	670	672	674	rVB	103073	85636	1.84%	0.214%
14	9.825	675	677	679	rVV	1526776	1316416	28.31%	3.294%
15	10.270	711	716	717	rBV3	121328	220336	4.74%	0.551%
16	10.488	731	735	738	rBV	65536	120320	2.59%	0.301%
17	10.613	743	746	749	rVV	2432394	2498339	53.73%	6.251%
18	10.739	752	757	763	rVB	220343	353506	7.60%	0.884%
19	10.933	772	774	776	rBV2	30042	55112	1.19%	0.138%
20	11.185	792	796	797	rBV	157356	162417	3.49%	0.406%
21	11.208	797	798	802	rVB	41776	57052	1.23%	0.143%
22	11.310	805	807	810	rVV2	796320	1350656	29.05%	3.379%
23	11.379	810	813	818	rVB2	65451	142259	3.06%	0.356%
24	11.539	825	827	831	rBV	218419	226807	4.88%	0.567%
25	11.608	831	833	837	rVB	88177	84304	1.81%	0.211%
26	11.916	858	860	865	rVB3	44098	69459	1.49%	0.174%
27	12.019	865	869	871	rBV	37498	49010	1.05%	0.123%
28	12.362	897	899	901	rBV	48431	79294	1.71%	0.198%
29	12.511	910	912	914	rBV	320144	312579	6.72%	0.782%
30	12.739	928	932	934	rBV	263739	378958	8.15%	0.948%
31	12.774	934	935	936	rVB	67399	50089	1.08%	0.125%
32	12.888	943	945	948	rBV	2277741	2793019	60.06%	6.988%
33	13.128	964	966	968	rVB2	120054	106655	2.29%	0.267%
34	13.471	994	996	997	rBV	131680	112790	2.43%	0.282%

LSC Area Percent Report

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Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

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-BF042716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.791	1022	1024	1029	rBV	183110	268685	5.78%	0.672%
36	13.939	1034	1037	1044	rVV2	600838	1080746	23.24%	2.704%
37	14.111	1050	1052	1054	rBV	60315	65457	1.41%	0.164%
38	14.328	1068	1071	1075	rBV4	22503	56596	1.22%	0.142%
39	14.419	1077	1079	1082	rBV2	68153	108072	2.32%	0.270%
40	14.648	1095	1099	1101	rBV4	20877	53149	1.14%	0.133%
41	14.694	1101	1103	1107	rVV2	83572	154177	3.32%	0.386%
42	14.785	1109	1111	1114	rVB2	33252	49074	1.06%	0.123%
43	14.945	1122	1125	1130	rBV	90909	199660	4.29%	0.500%
44	15.025	1130	1132	1135	rBV2	130420	167257	3.60%	0.418%
45	15.219	1147	1149	1152	rBV	54784	71554	1.54%	0.179%
46	15.277	1152	1154	1157	rBV	60472	81455	1.75%	0.204%
47	15.334	1157	1159	1162	rBV	553390	813994	17.51%	2.037%
48	15.780	1195	1198	1201	rBV	193656	279256	6.01%	0.699%
49	16.728	1278	1281	1284	rVV	134318	256550	5.52%	0.642%
50	18.008	1390	1393	1400	rVB7	19331	51307	1.10%	0.128%

Sum of corrected areas: 39969209

LSC Report - Integrated Chromatogram

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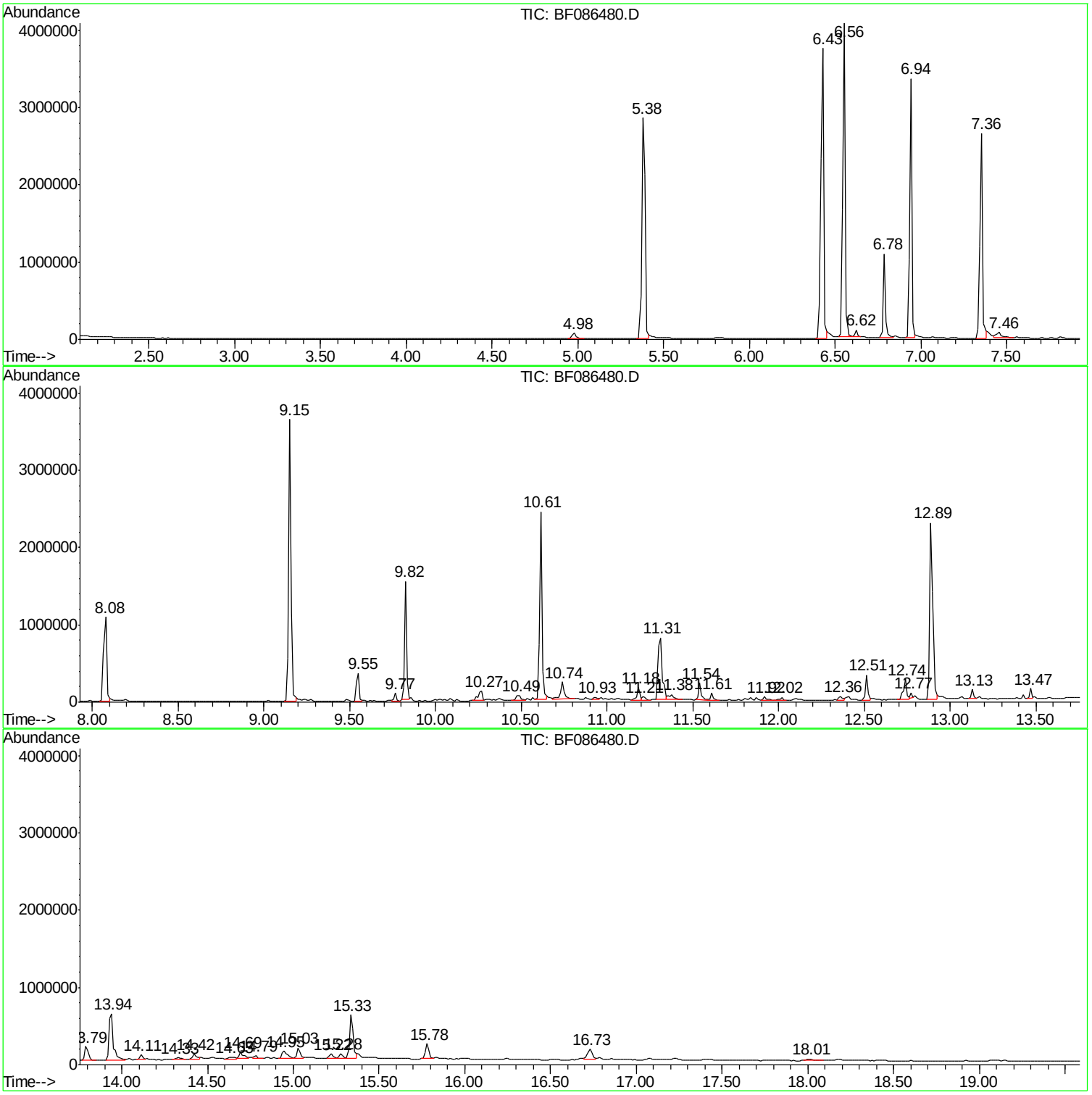
Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086480.D
Acq On : 28 Apr 2016 23:20
Operator : UM/SJ
Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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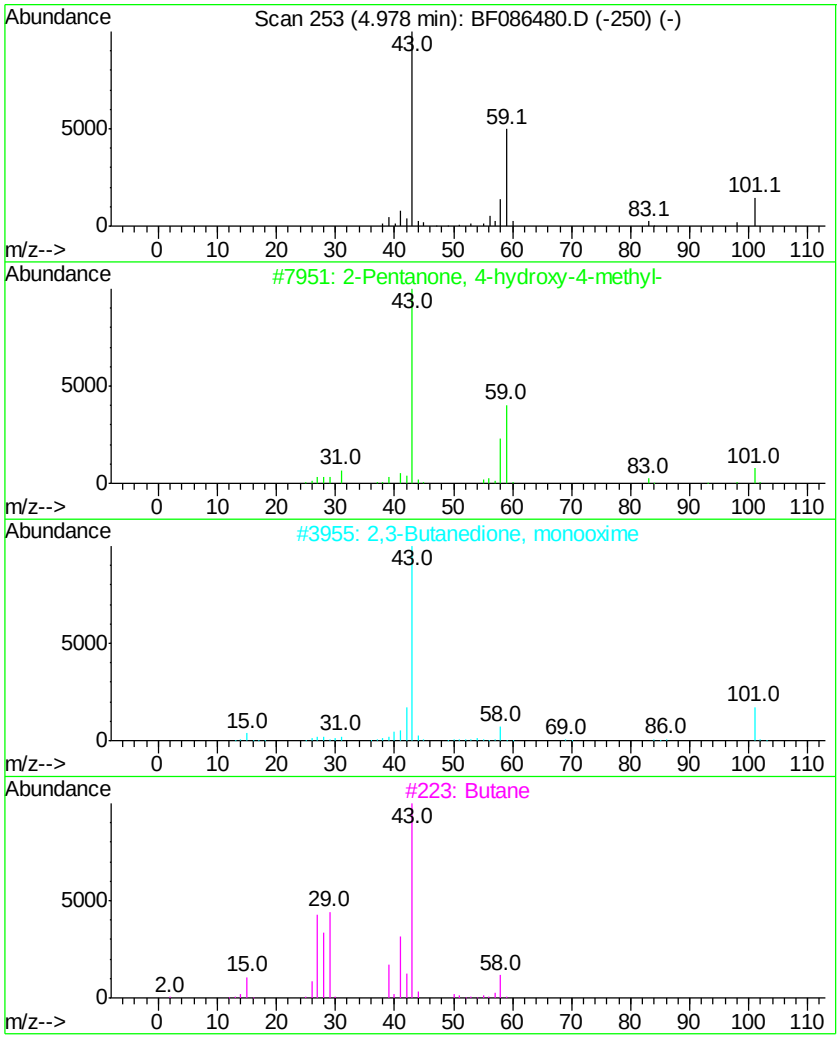
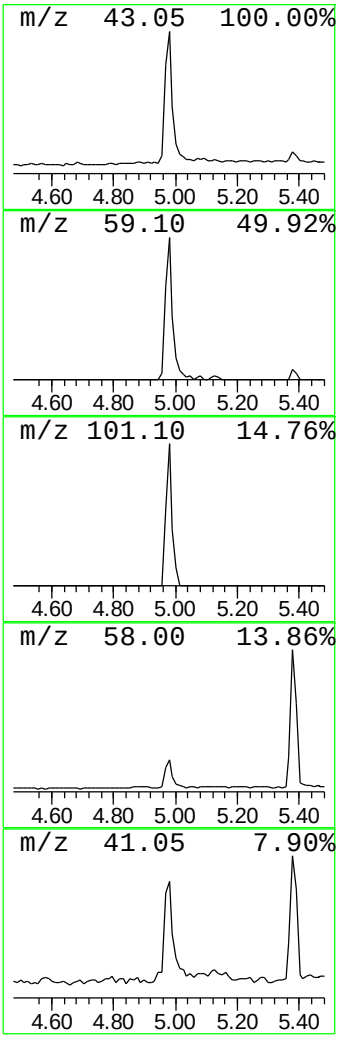
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	2.26 ng	114528	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Butane	58	C4H10	000106-97-8	9
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
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Sample : H2654-09
Misc :
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Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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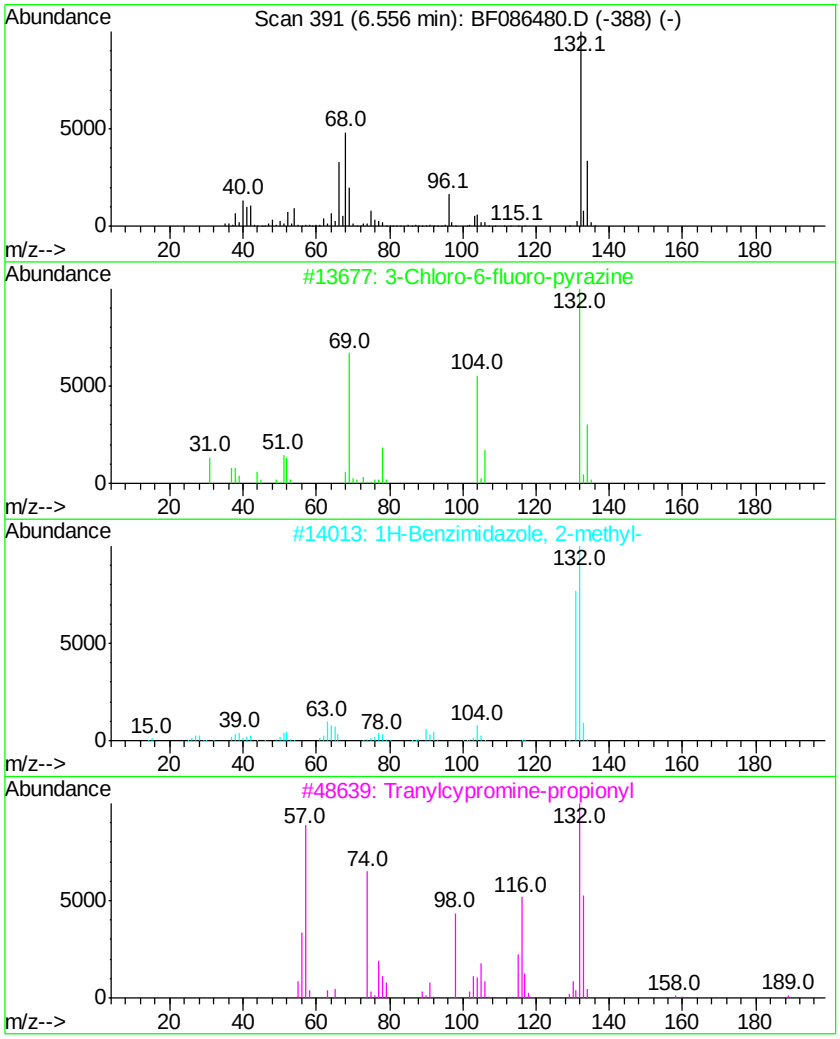
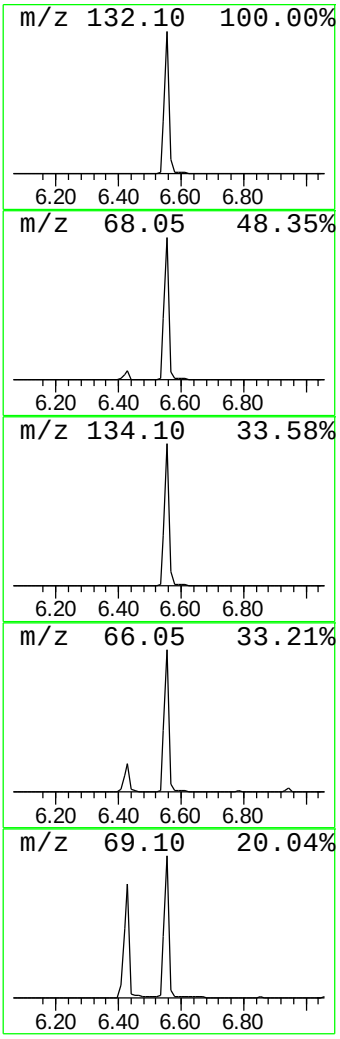
Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	81.76 ng	4141170	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





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Acq On : 28 Apr 2016 23:20
Operator : UM/SJ
Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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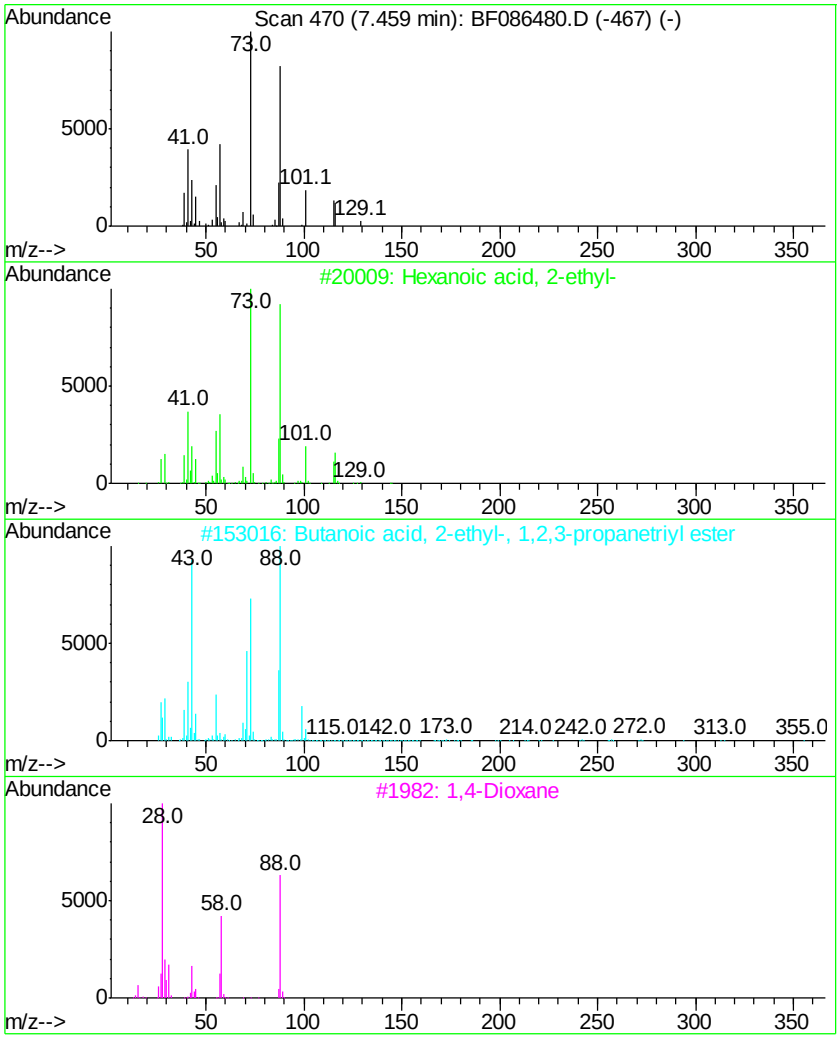
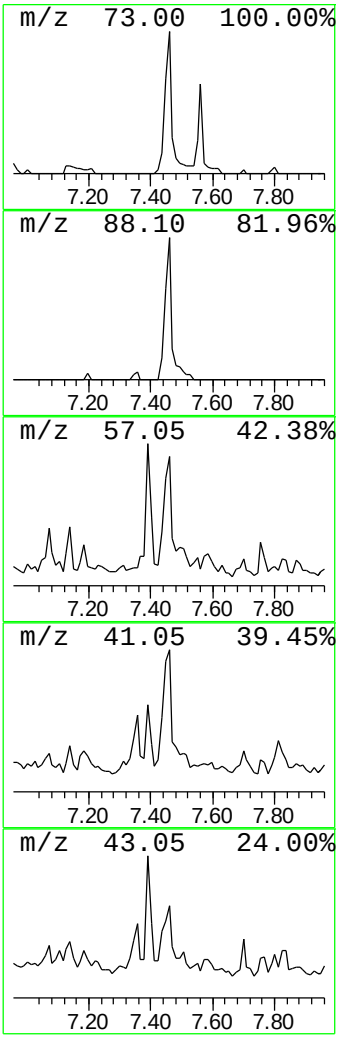
Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	2.53 ng	160407	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
3	1,4-Dioxane	88	C4H8O2	000123-91-1	38
4	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	36
5	Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	33





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Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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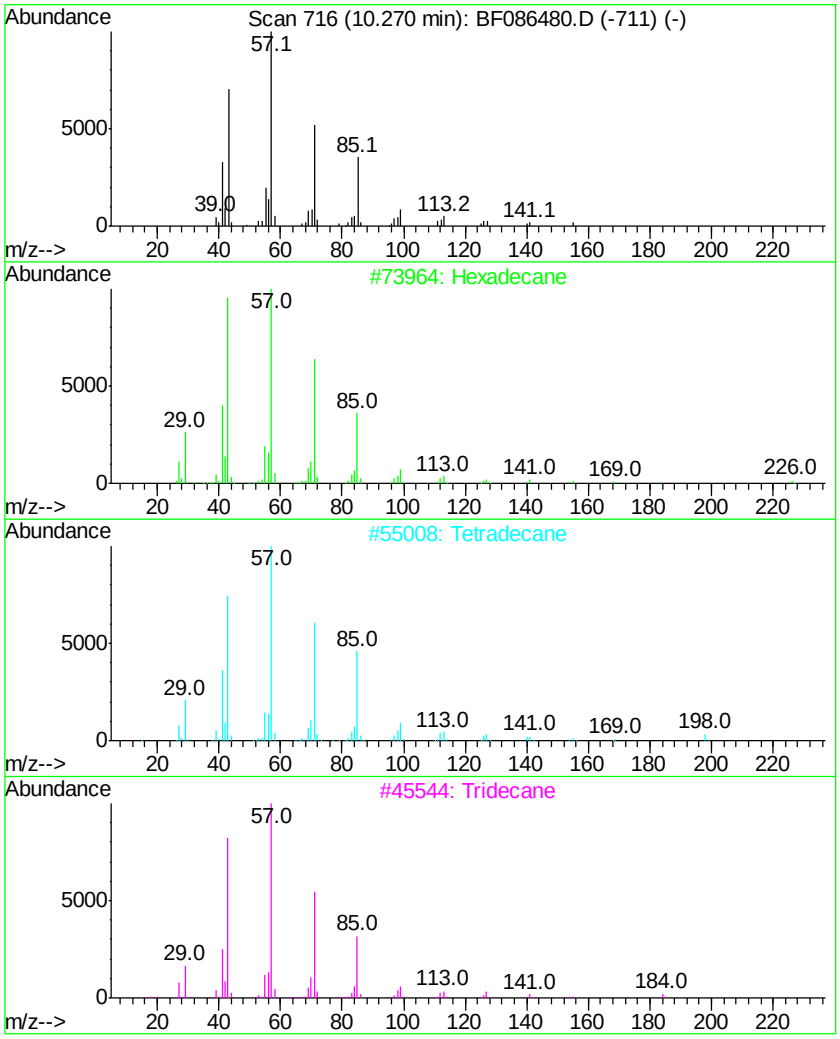
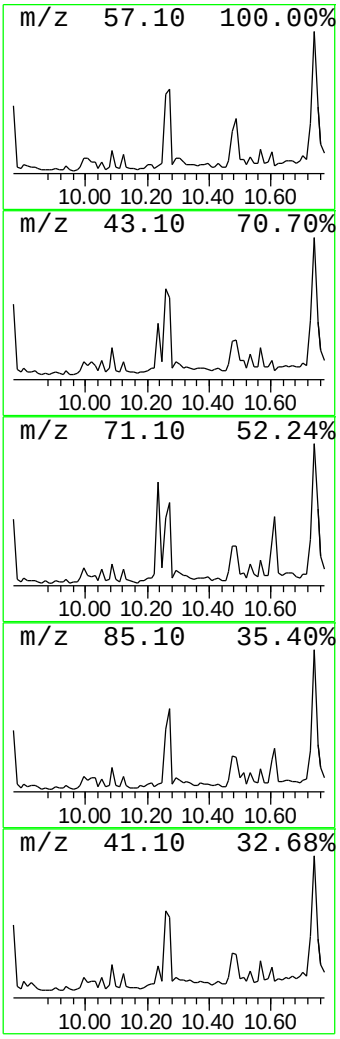
Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	3.35 ng	220336	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	91
3	Tridecane	184	C13H28	000629-50-5	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tetracosane	338	C24H50	000646-31-1	86





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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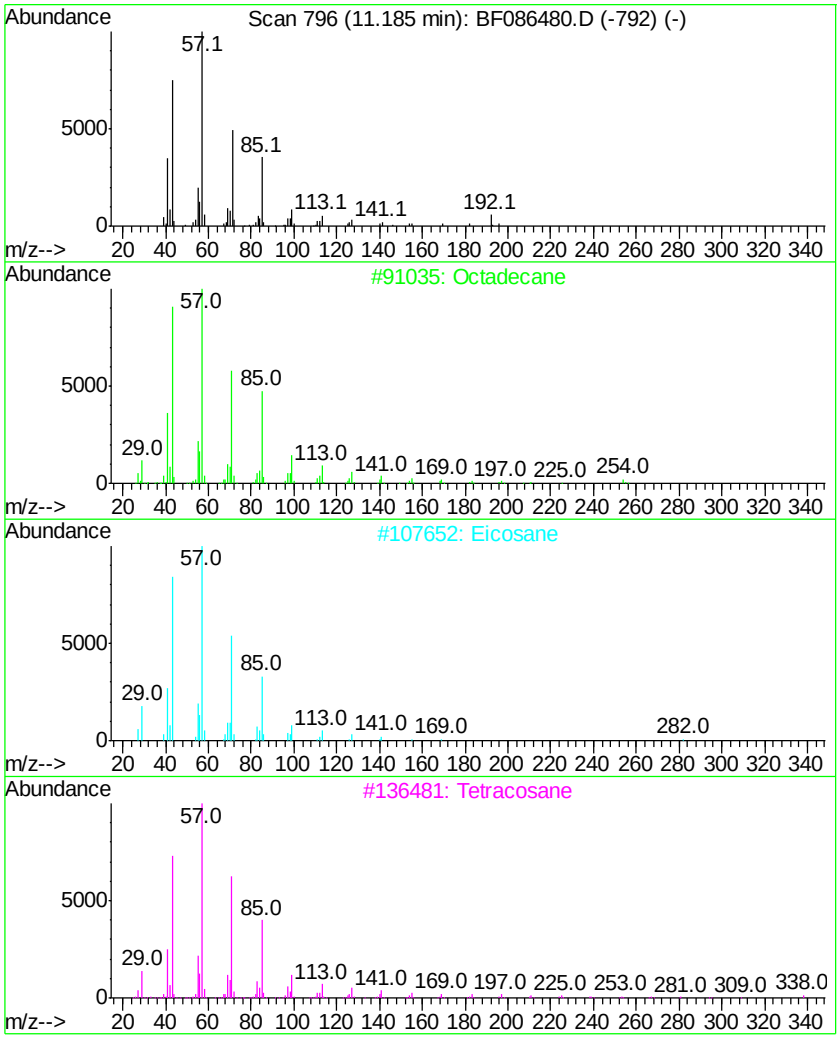
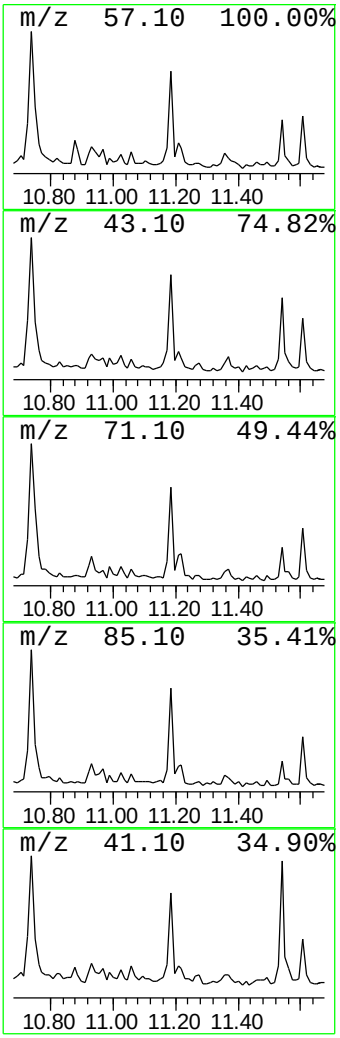
Peak Number 7 Octadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	2.41 ng	162417	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	83
2	Eicosane	282	C20H42	000112-95-8	83
3	Tetracosane	338	C24H50	000646-31-1	80
4	Pentadecane	212	C15H32	000629-62-9	80
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80





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Sample : H2654-09
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ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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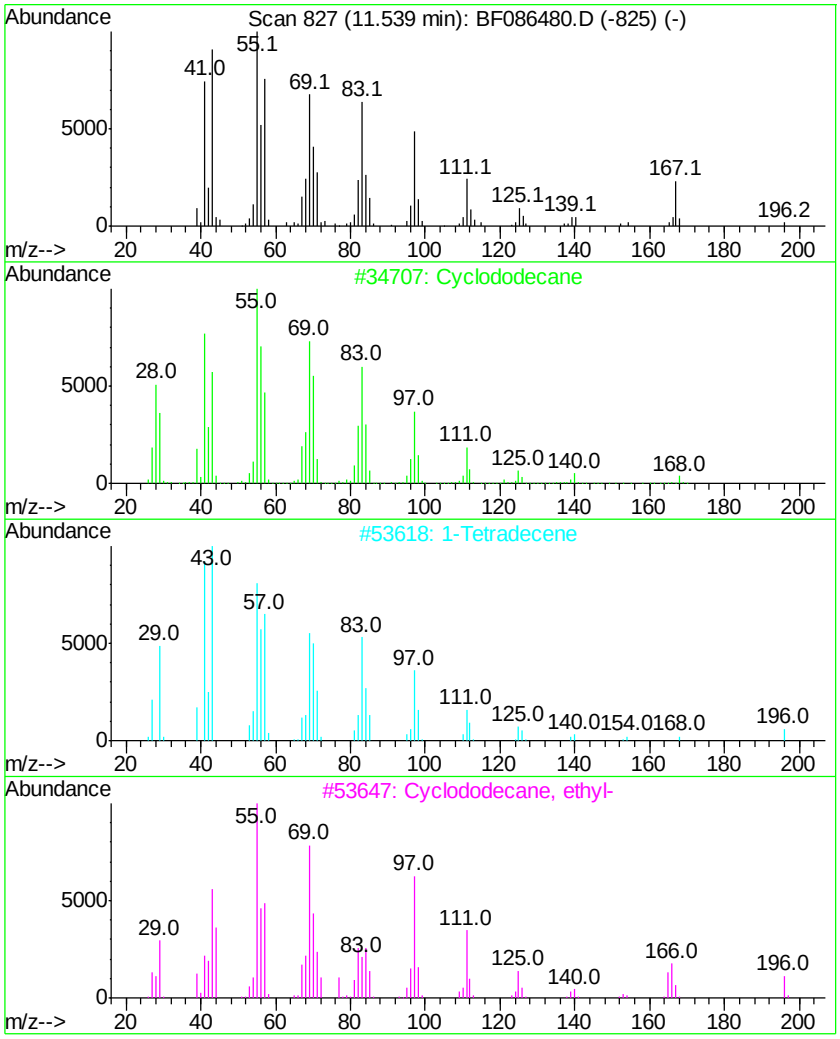
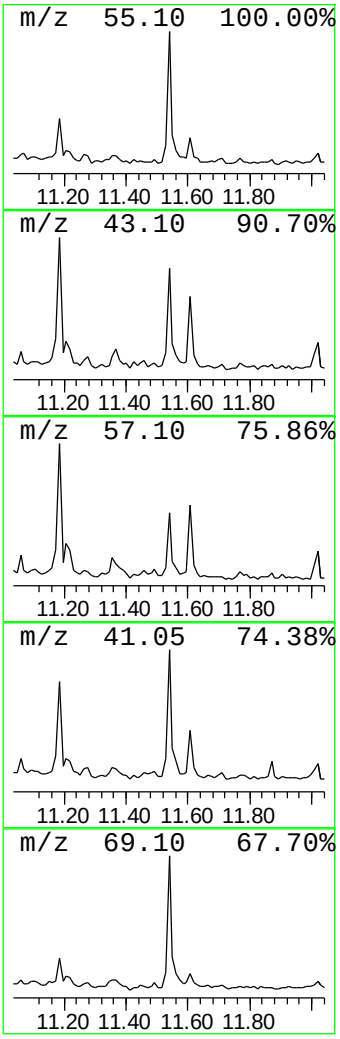
Peak Number 8 Cyclododecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	3.36 ng	226807	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecane	168	C12H24	000294-62-2	97
2	1-Tetradecene	196	C14H28	001120-36-1	94
3	Cyclododecane, ethyl-	196	C14H28	028981-49-9	93
4	5-Tetradecene, (Z)-	196	C14H28	041446-62-2	91
5	1-Hexadecene	224	C16H32	000629-73-2	90





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Misc :
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Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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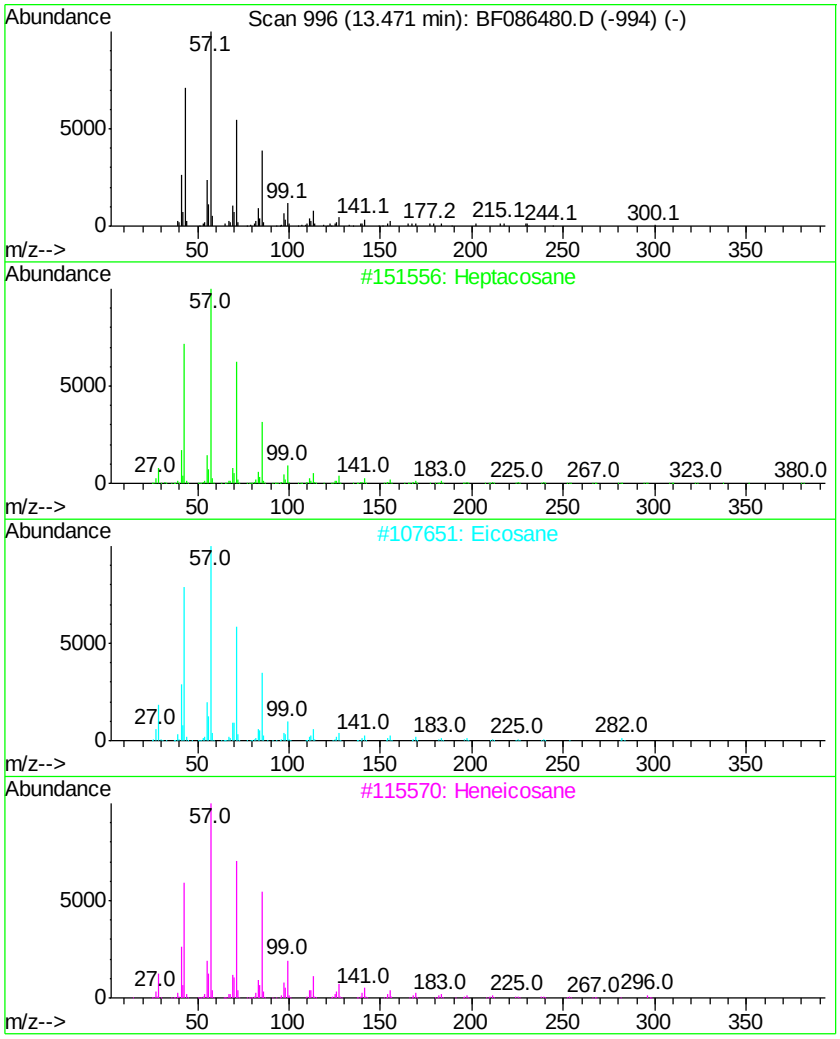
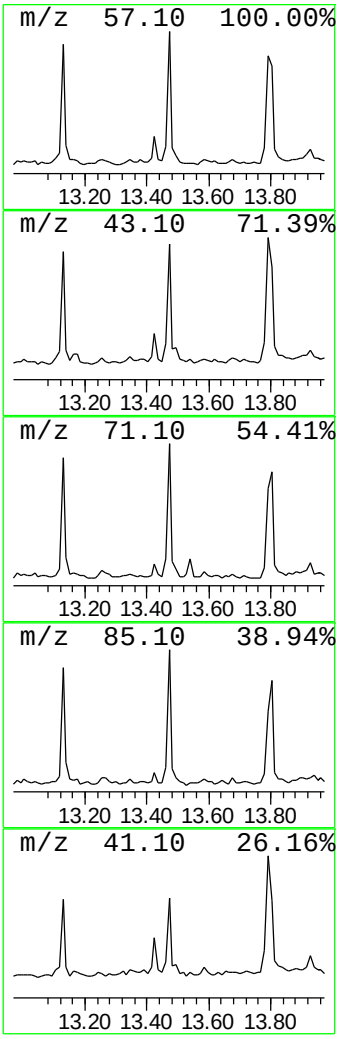
Peak Number 9 Heptacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	2.09 ng	112790	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Eicosane	282	C20H42	000112-95-8	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086480.D
Acq On : 28 Apr 2016 23:20
Operator : UM/SJ
Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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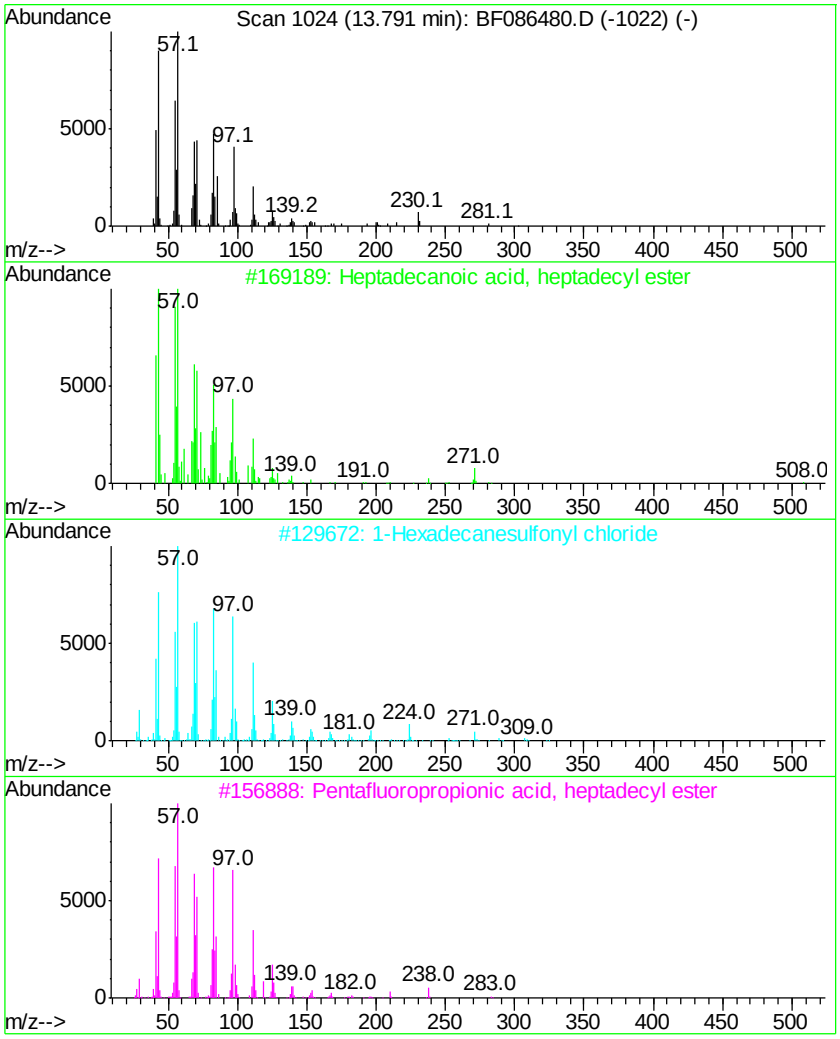
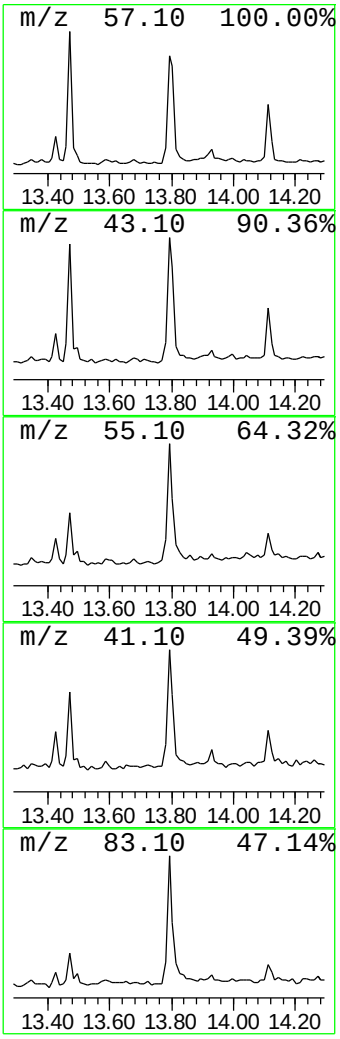
Peak Number 10 Heptadecanoic acid, heptade... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	4.97 ng	268685	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	91
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	83





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Data File : BF086480.D
Acq On : 28 Apr 2016 23:20
Operator : UM/SJ
Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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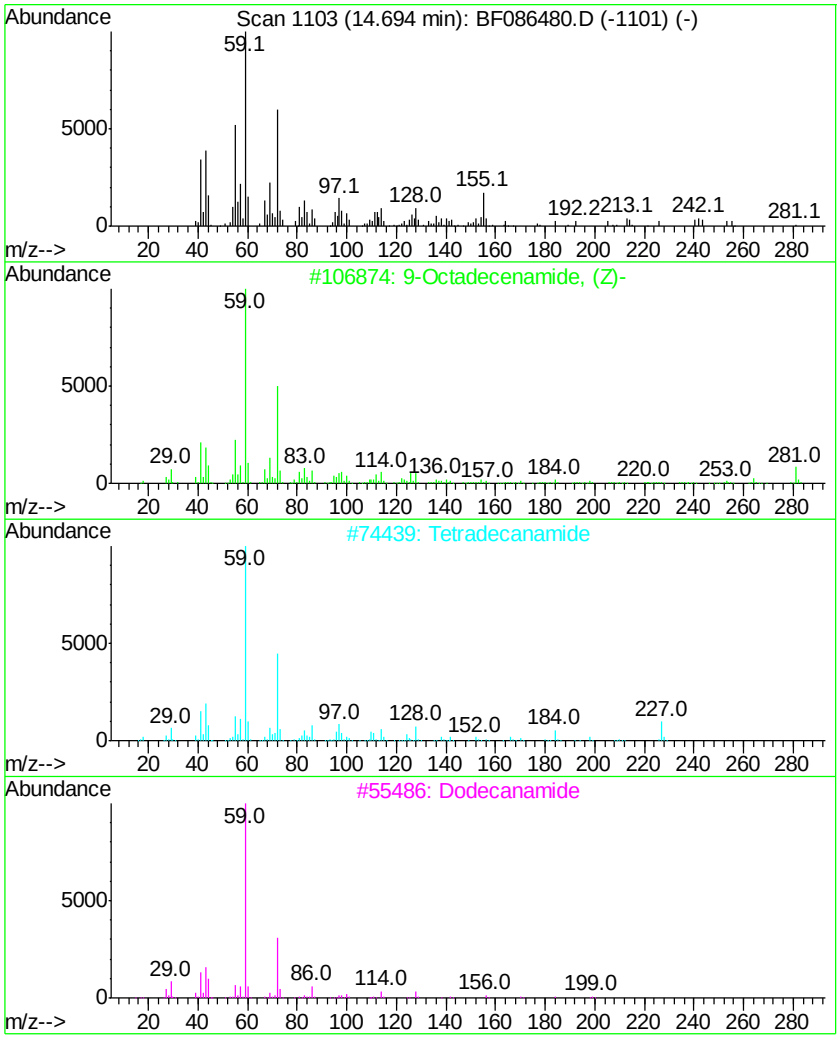
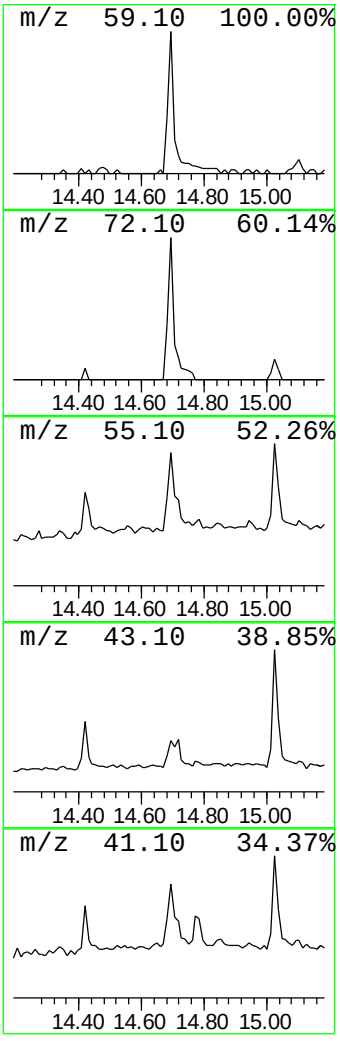
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	3.79 ng	154177	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2	Tetradecanamide	227	C14H29NO	000638-58-4	72
3	Dodecanamide	199	C12H25NO	001120-16-7	53
4	d-Glucosamine	179	C6H13NO5	000090-77-7	53
5	Hexadecanamide	255	C16H33NO	000629-54-9	50





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Data File : BF086480.D
Acq On : 28 Apr 2016 23:20
Operator : UM/SJ
Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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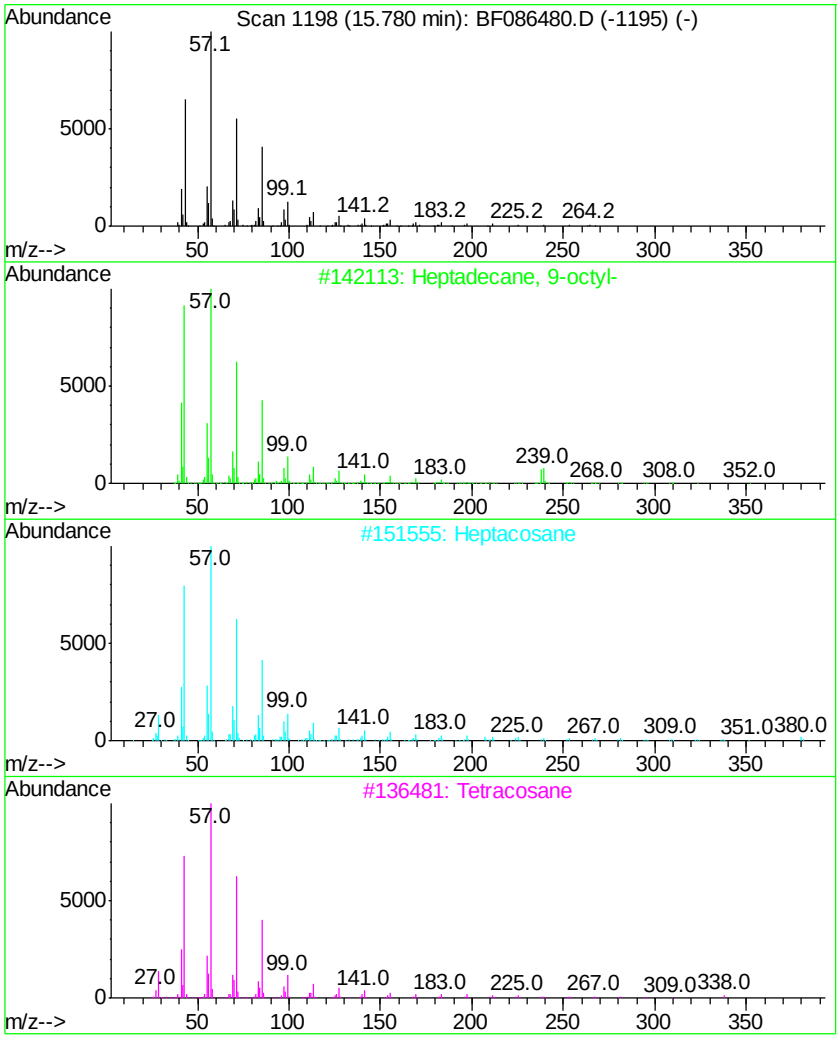
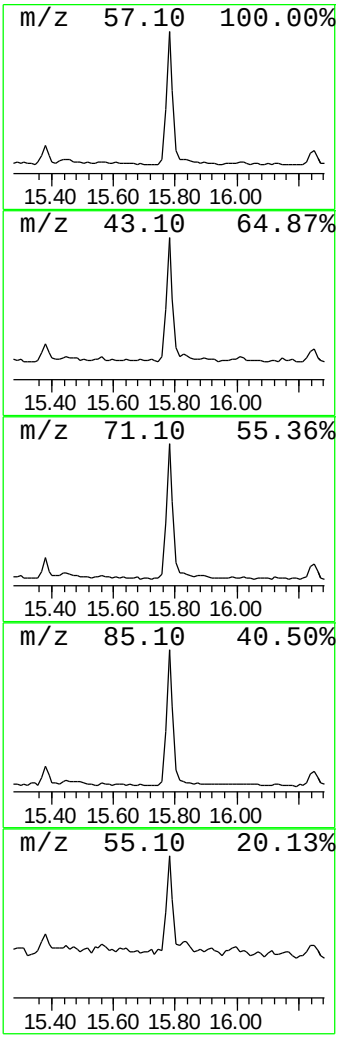
Peak Number 13 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	6.86 ng	279256	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Octacosane	394	C28H58	000630-02-4	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042816\
Data File : BF086480.D
Acq On : 28 Apr 2016 23:20
Operator : UM/SJ
Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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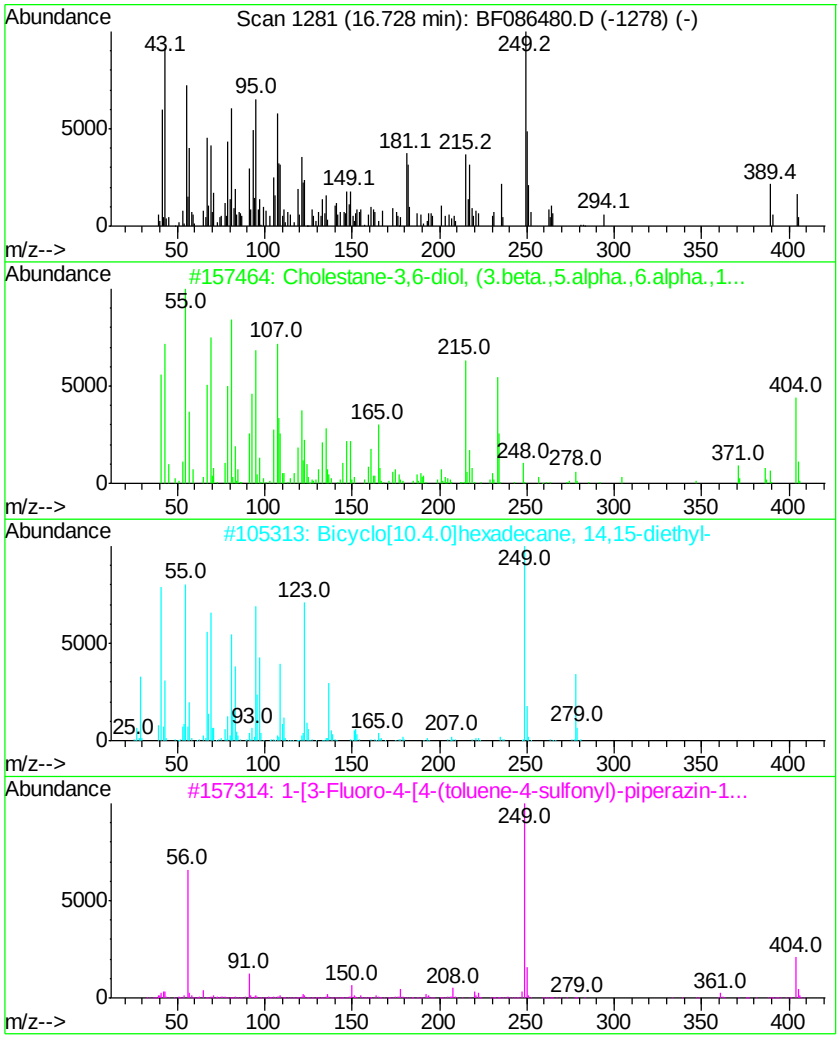
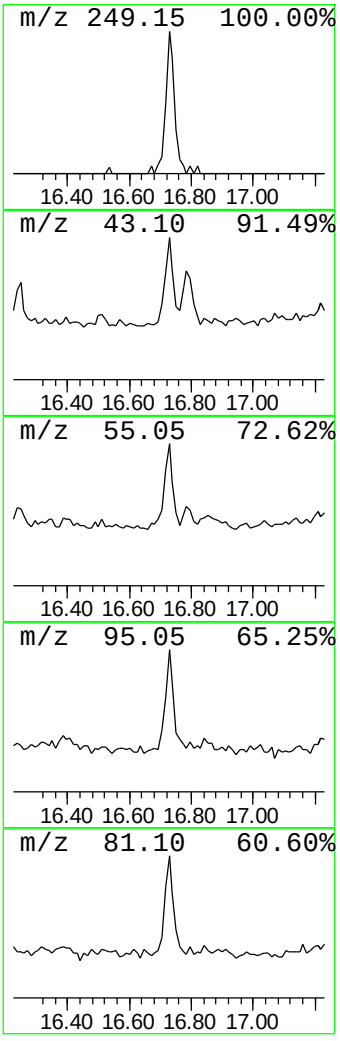
Peak Number 14 unknown16.73 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.73	6.30 ng	256550	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestane-3,6-diol, (3.beta.,5....	404	C27H48O2	041083-77-6	35
2	Bicyclo[10.4.0]hexadecane, 14,15...	278	C20H38	1000155-81-5	25
3	1-[3-Fluoro-4-[4-(toluene-4-sulf...	404	C21H25FN2O3S	333751-65-8	25
4	2-Amino-4,6-dimethyl-5-iodopyrim...	249	C6H8IN3	002033-47-8	22
5	10H-Phenothiazin-3-ol, 2-chloro-	249	C12H8ClNOS	016770-99-3	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042816\
Data File : BF086480.D
Acq On : 28 Apr 2016 23:20
Operator : UM/SJ
Sample : H2654-09
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 26WARD-2A-CS-18(6-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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...	4.98	2.3	ng	114528	1	6.78	1013010	20.0
unknown6.56	6.56	81.8	ng	4141170	1	6.78	1013010	20.0
Hexanoic acid, 2-...	7.46	2.5	ng	160407	2	8.08	1265750	20.0
Hexadecane	10.27	3.4	ng	220336	3	9.82	1316420	20.0
Octadecane	11.18	2.4	ng	162417	4	11.31	1350660	20.0
Cyclododecane	11.54	3.4	ng	226807	4	11.31	1350660	20.0
Heptacosane	13.47	2.1	ng	112790	5	13.94	1080750	20.0
Heptadecanoic aci...	13.79	5.0	ng	268685	5	13.94	1080750	20.0
9-Octadecenamide,...	14.69	3.8	ng	154177	6	15.33	813994	20.0
Heptadecane, 9-oc...	15.78	6.9	ng	279256	6	15.33	813994	20.0
unknown16.73	16.73	6.3	ng	256550	6	15.33	813994	20.0