LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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	4.910	244	247	264	rBV	162342	423047	6.73%	0.776%
2	5.310	280	282	285	rBV	4389364	5182780	82.51%	9.501%
3	6.361	371	374	377	rBV	4115789	6091761	96.98%	11.168%
4	6.476	382	384	387	rVV	4882524	5426784	86.39%	9.949%
5	6.704	402	404	406	rBV	1273789	1267639	20.18%	2.324%
6	6.864	415	418	420	rBV	3143121	4208616	67.00%	7.715%
7	7.276	451	454	456	rBV	3444891	3759533	59.85%	6.892%
8	7.984	514	516	519	rBV	1256415	1600956	25.49%	2.935%
9	9.070	607	611	613	rBV	5538103	6281563	100.00%	11.516%
10	9.470	643	646	648	rBV	812442	755538	12.03%	1.385%
11	9.676	662	664	667	rBV	119832	114601	1.82%	0.210%
12	9.733	667	669	672	rBV	1285441	1753809	27.92%	3.215%
13	10.179	704	708	710	rBV	286202	271127	4.32%	0.497%
14	10.396	724	727	730	rBV	97291	159406	2.54%	0.292%
15	10.476	730	734	736	rBV2	90959	156489	2.49%	0.287%
16	10.533	736	739	741	rBV	3547922	4268707	67.96%	7.826%
17	10.647	747	749	756	rVB	325150	387410	6.17%	0.710%
18	11.093	786	788	790	rBV	145363	141260	2.25%	0.259%
19	11.219	797	799	801	rBV	1821396	1710821	27.24%	3.136%
20	11.756	845	846	852	rVB2	325417	462432	7.36%	0.848%
21	12.431	903	905	906	rBV	45348	88236	1.40%	0.162%
22	12.465	906	908	913	rVV	79922	164798	2.62%	0.302%
23	12.545	913	915	919	rVV	312667	381724	6.08%	0.700%
24	12.808	935	938	940	rBV	5054146	5447754	86.73%	9.987%
25	13.711	1014	1017	1024	rBV	162591	229102	3.65%	0.420%
26	13.848	1026	1029	1031	rBV	1124382	1289774	20.53%	2.364%
27	14.351	1068	1073	1077	rBV2	53202	142815	2.27%	0.262%
28	14.682	1100	1102	1104	rVB2	82527	76663	1.22%	0.141%
29	14.922	1120	1123	1125	rBV	54980	65215	1.04%	0.120%
30	15.117	1137	1140	1143	rBV	84566	110785	1.76%	0.203%
31	15.219	1147	1149	1152	rVV	611773	931666	14.83%	1.708%
32	15.311	1155	1157	1163	rVB6	30883	75380	1.20%	0.138%
33	15.642	1183	1186	1189	rVB	52223	89236	1.42%	0.164%
34	18.088	1395	1400	1409	rVB2	160691	438203	6.98%	0.803%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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	18.294	1413	1418	1423	rVB	228200	592184	9.43%	1.086%

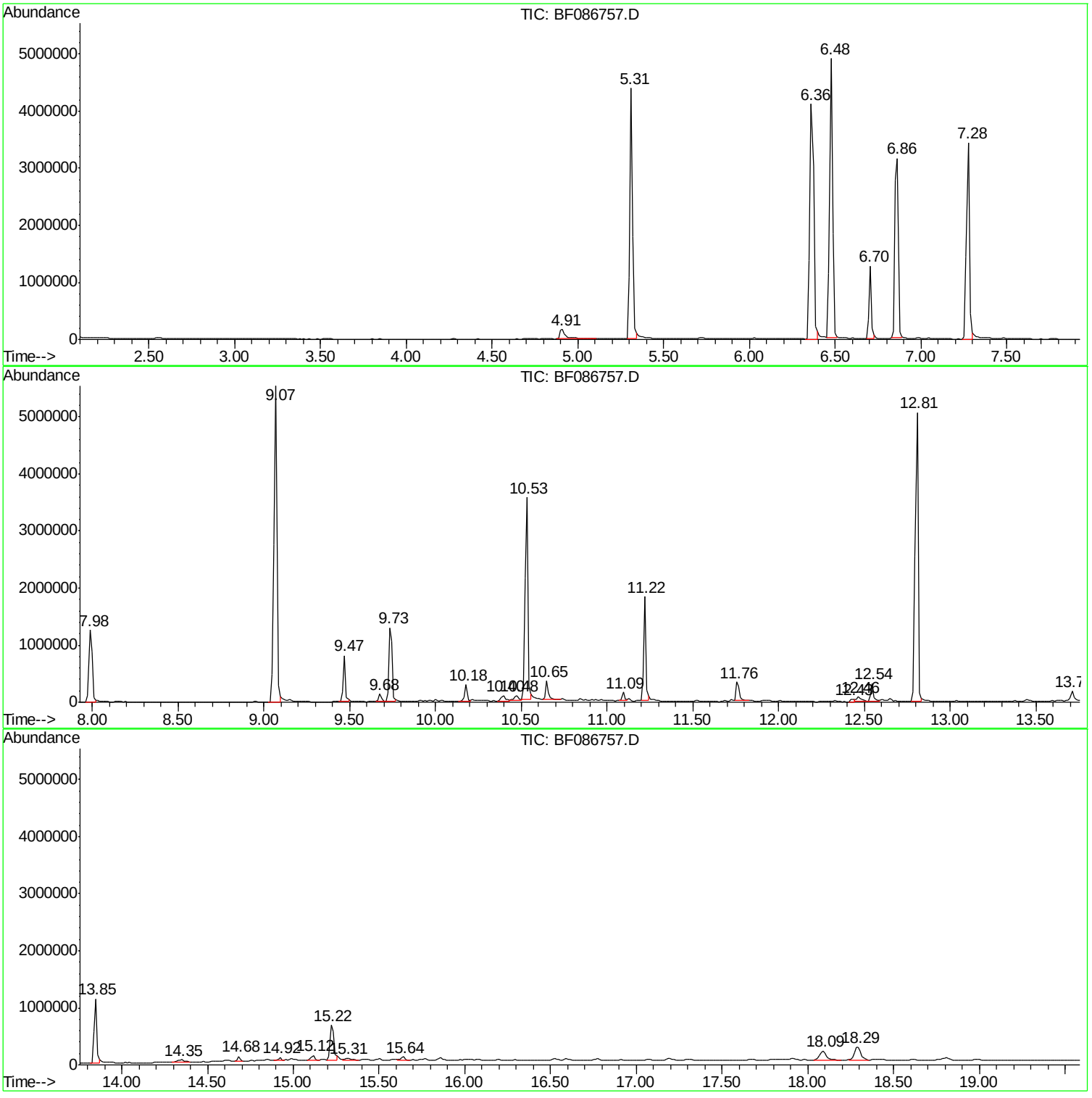
Sum of corrected areas: 54547814

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
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Instrument : BNA_F
ClientSampleId : SS1

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

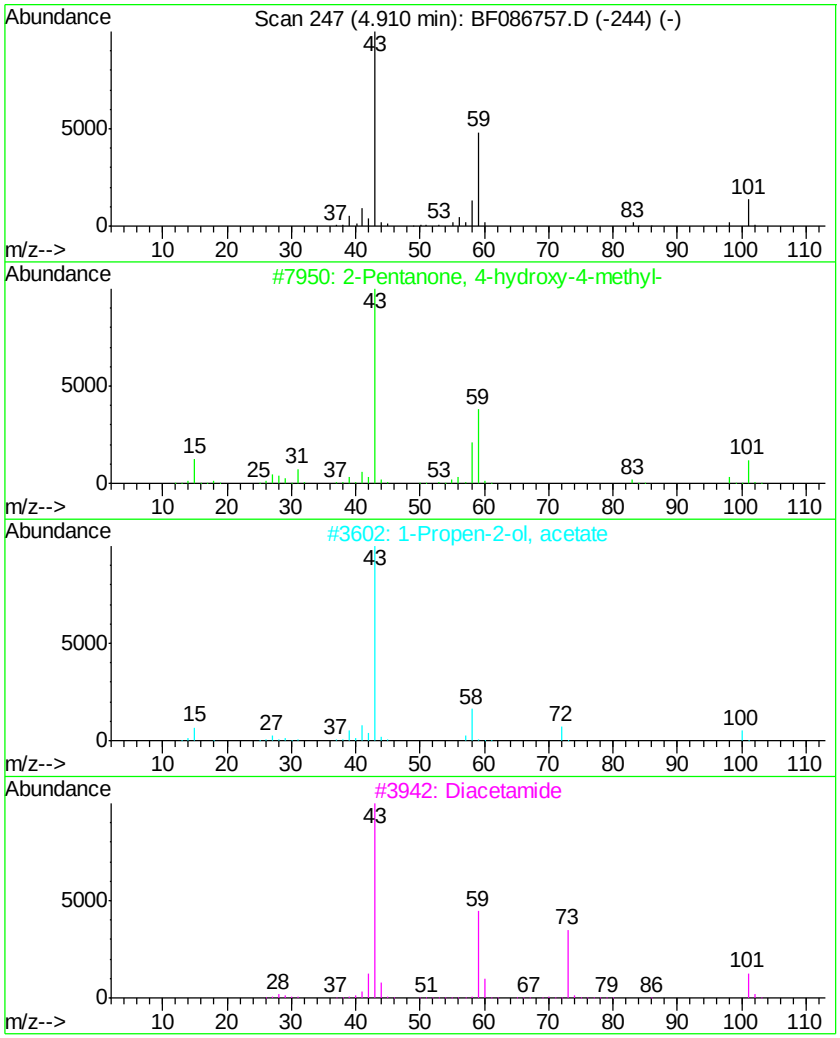
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

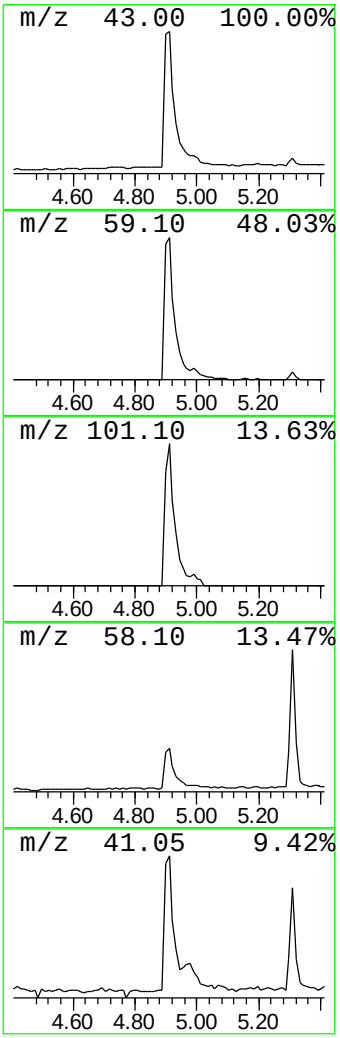
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	13.35 ng	423047	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	dl-4-Amino-3-hydroxybutyric acid	119	C4H9NO3	000352-21-6	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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

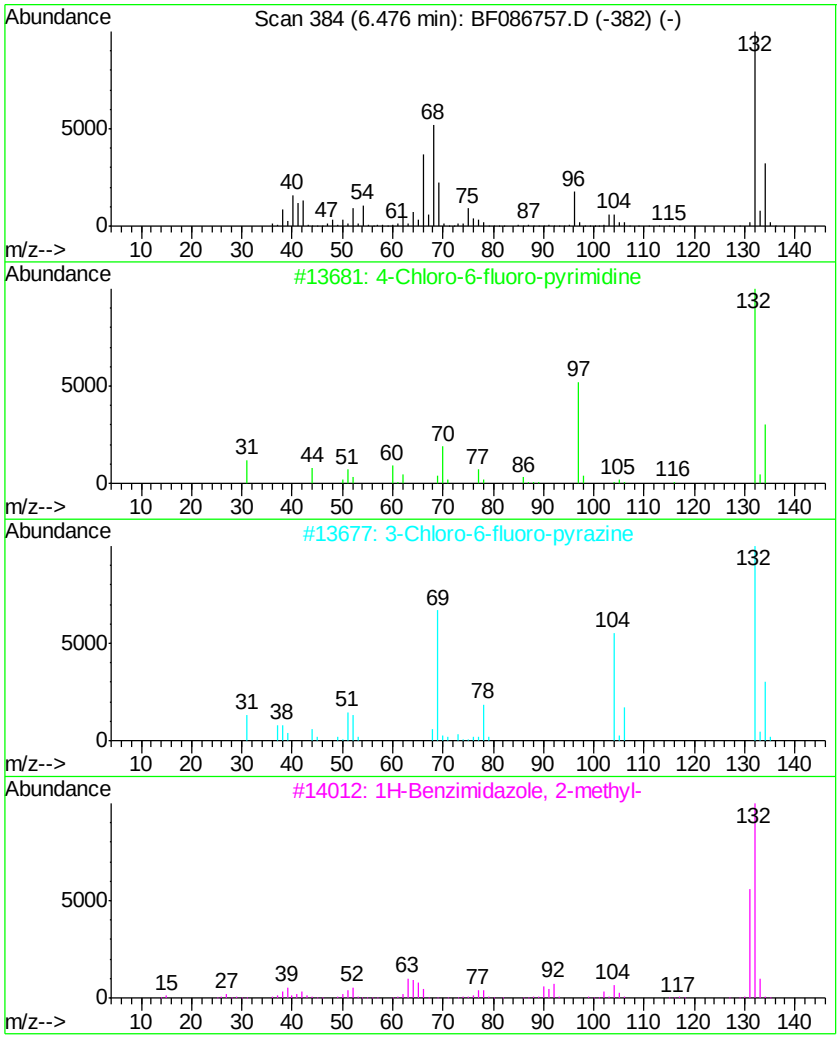
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

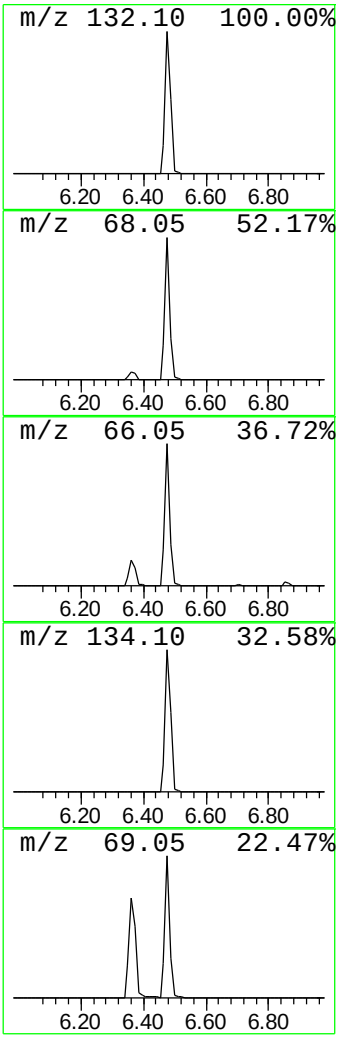
****

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	171.24 ng	5426780	1,4-Dichlorobenzene-d4	6.70

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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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

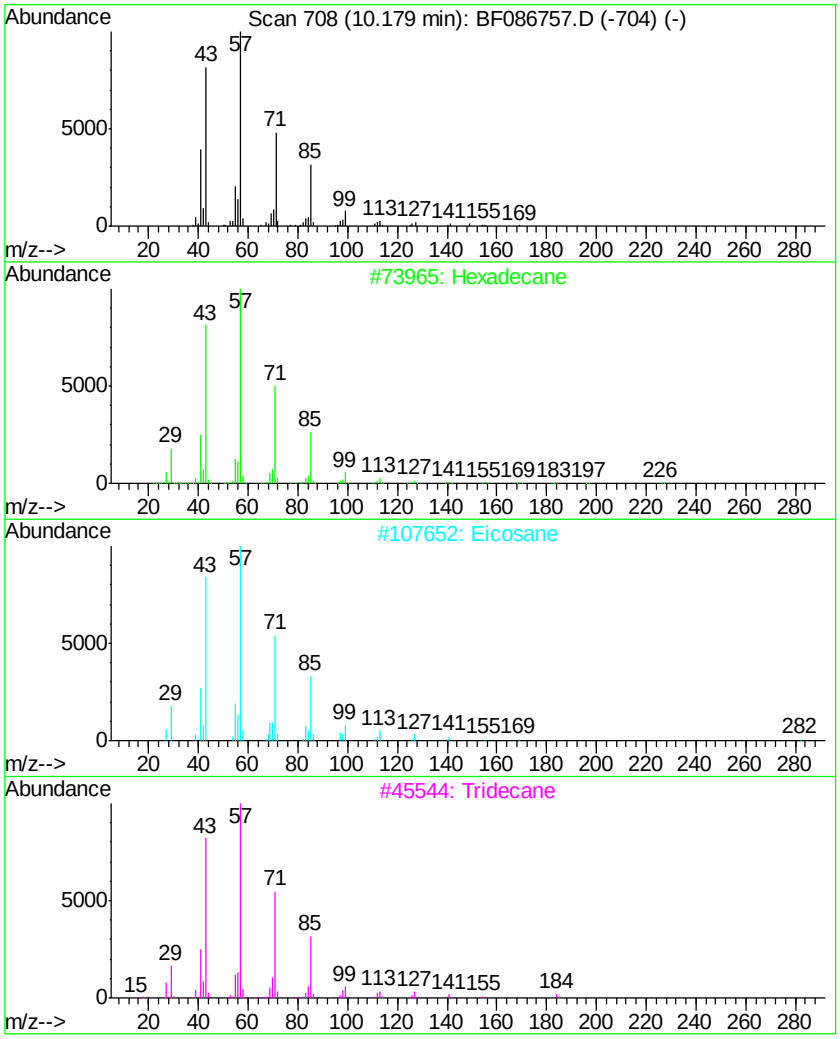
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

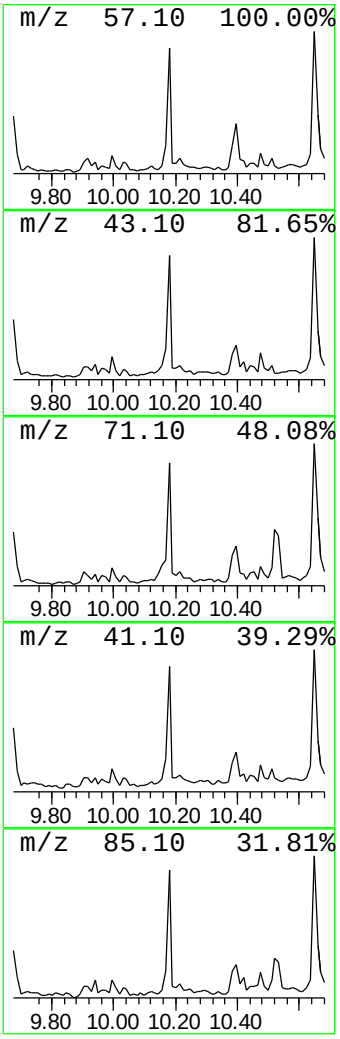
****

Peak Number 4 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	6.18 ng	271127	Acenaphthene-d10	9.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Decane, 3-bromo-	220	C10H21Br	030571-71-2	64
5	2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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

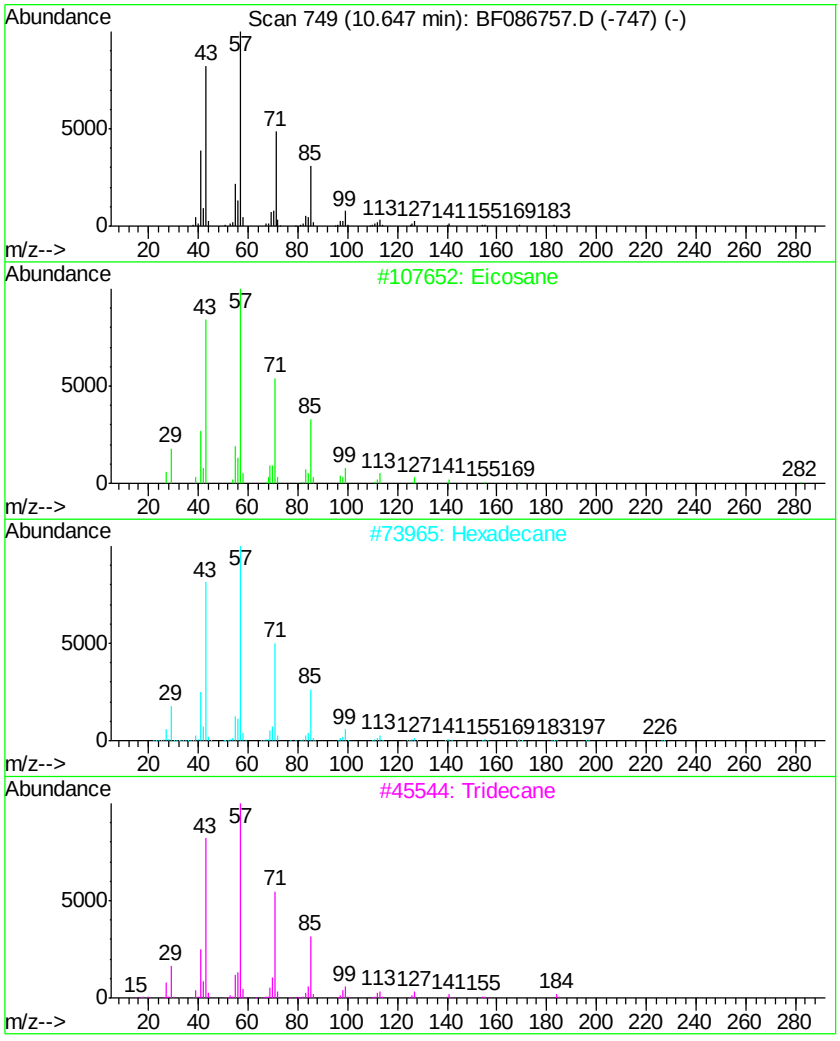
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

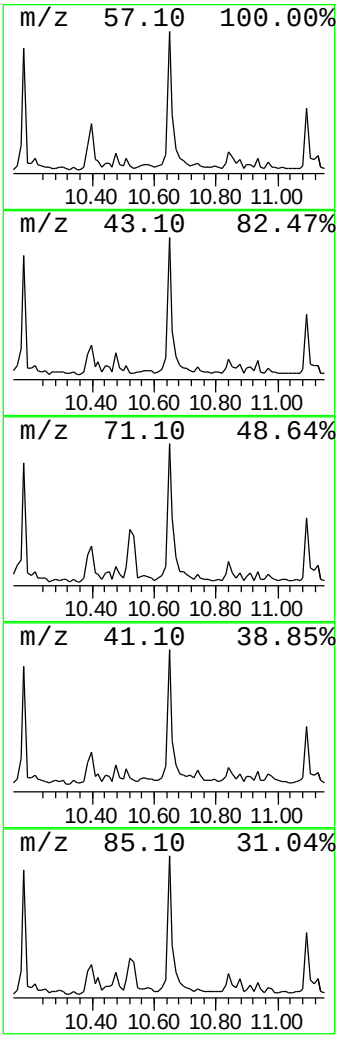
****

Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	9.06 ng	387410	Phenanthrene-d10	11.22

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	Tridecane	184	C13H28	000629-50-5	90
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	90
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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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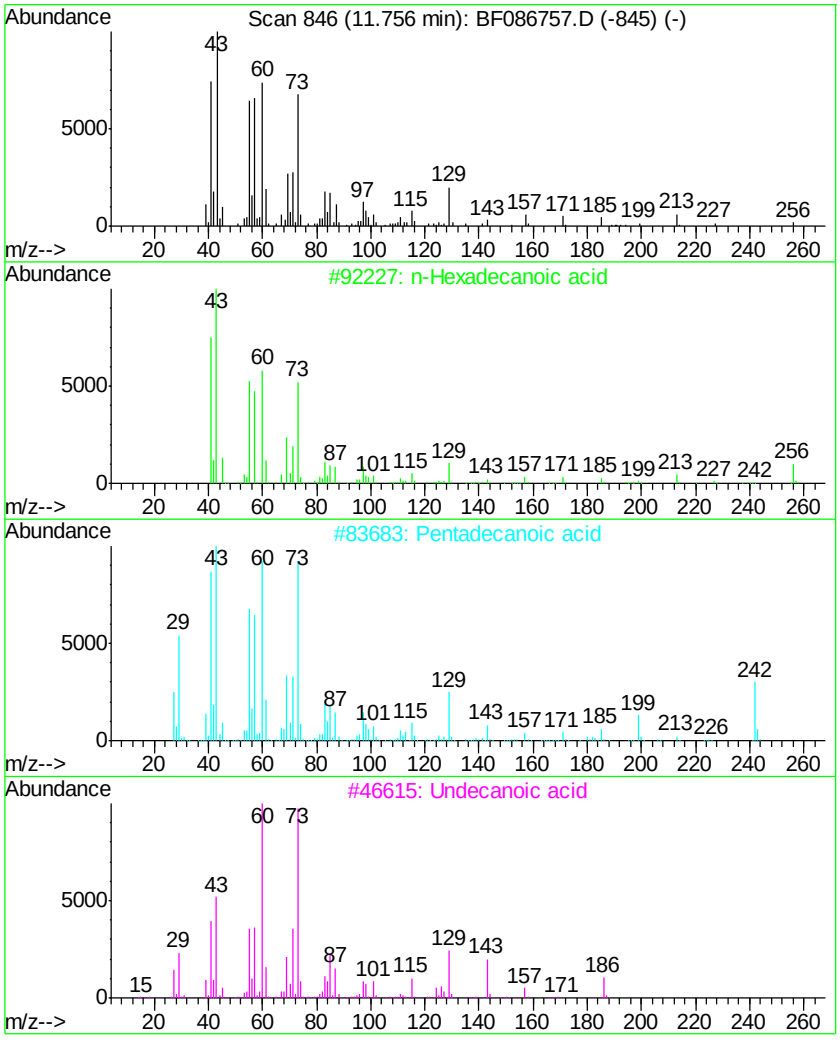
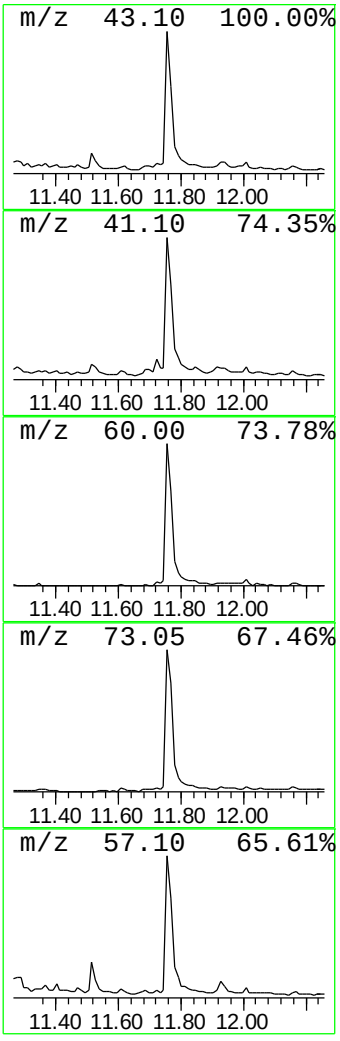
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	10.81 ng	462432	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	78
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5	n-Decanoic acid	172	C10H20O2	000334-48-5	74





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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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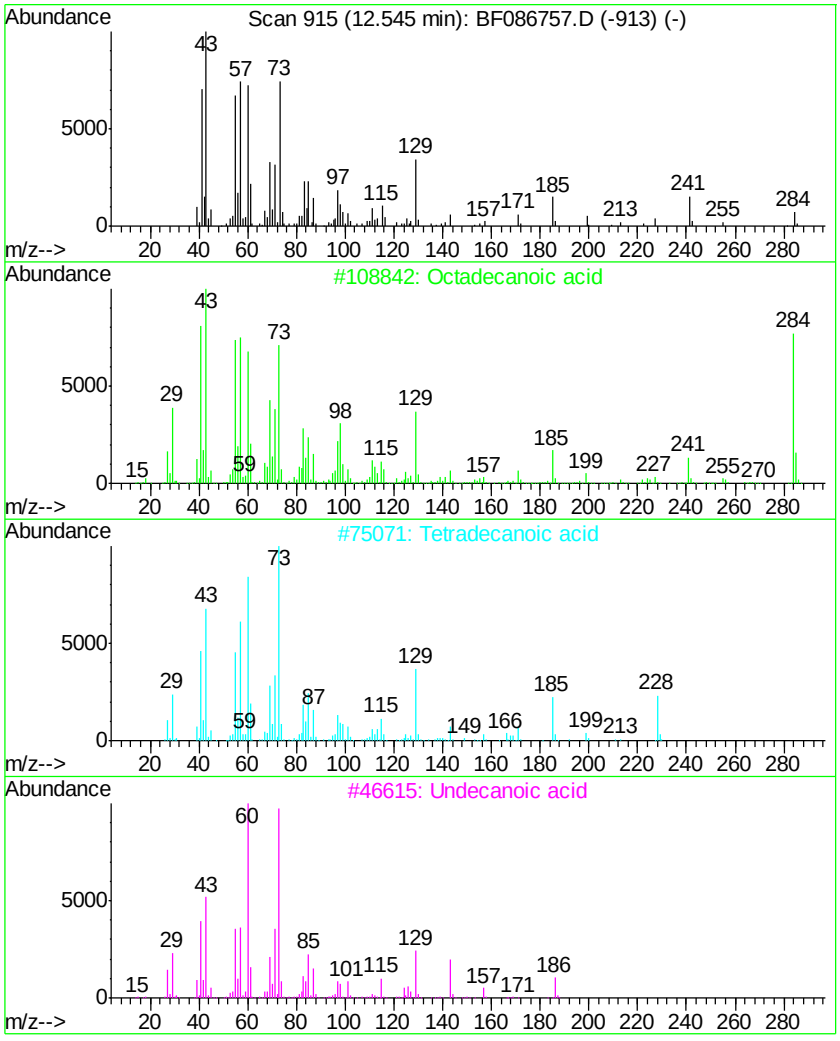
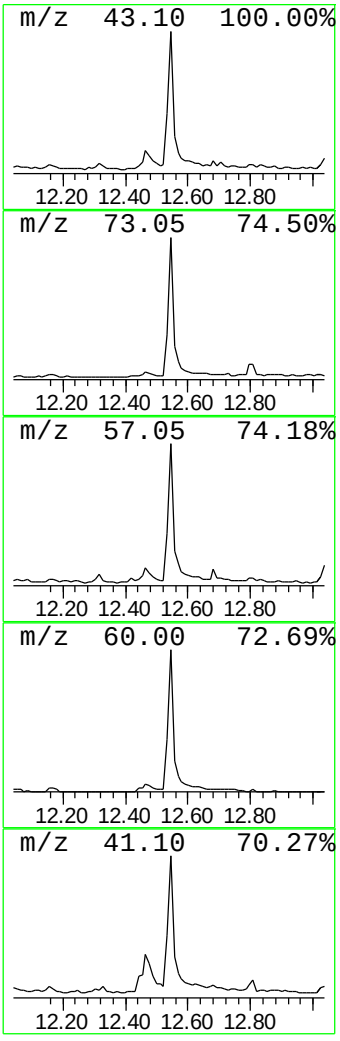
Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	11.84 ng	381724	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





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Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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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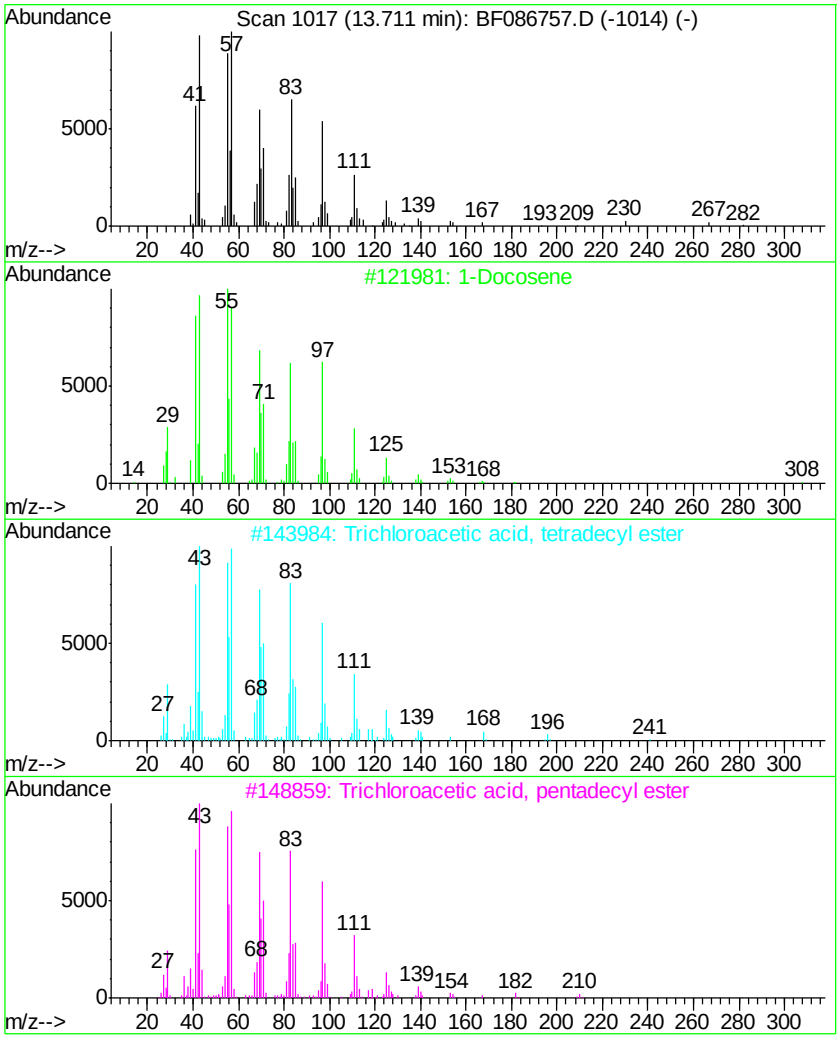
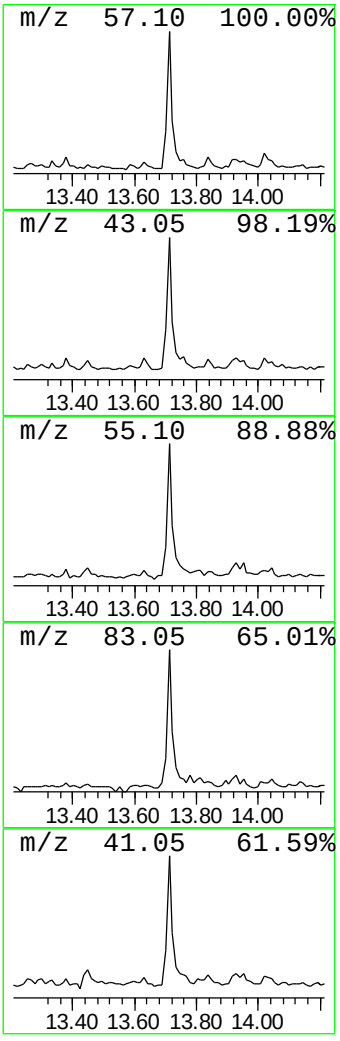
Peak Number 8 1-Docosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	7.11 ng	229102	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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Misc :
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Instrument : BNA_F
ClientSampleId : SS1

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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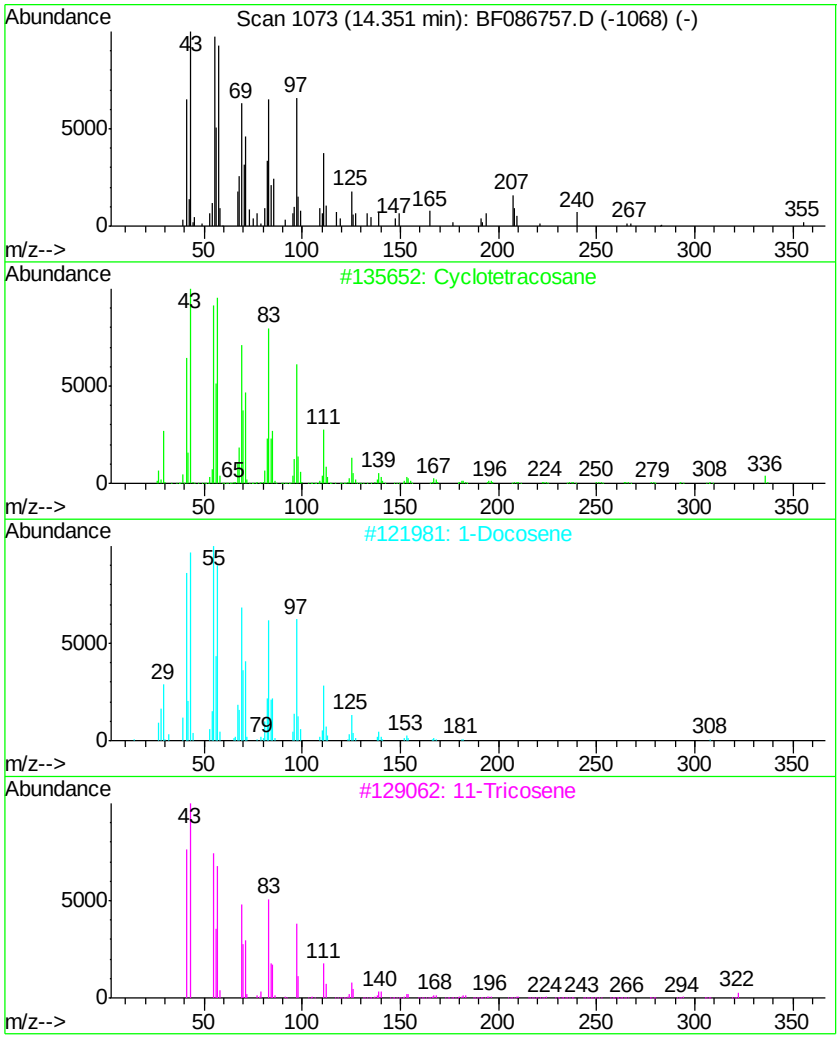
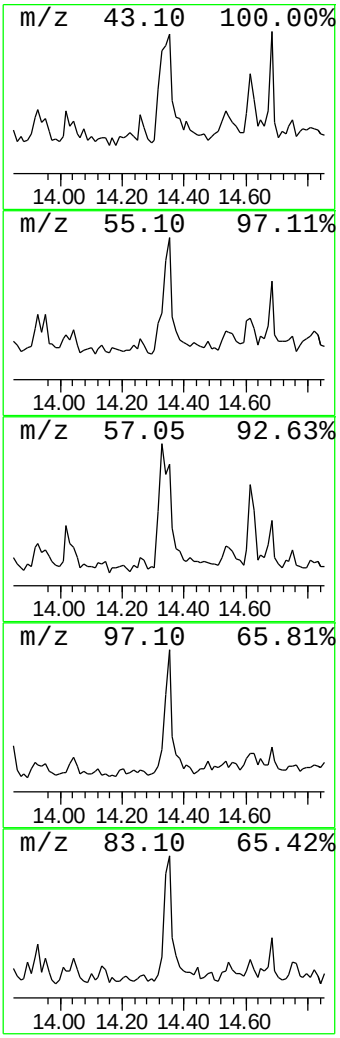
Peak Number 9 Cyclotetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	4.43 ng	142815	Chrysene-d12	13.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	90
2	1-Docosene	308	C22H44	001599-67-3	90
3	11-Tricosene	322	C23H46	052078-56-5	87
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	81
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	81





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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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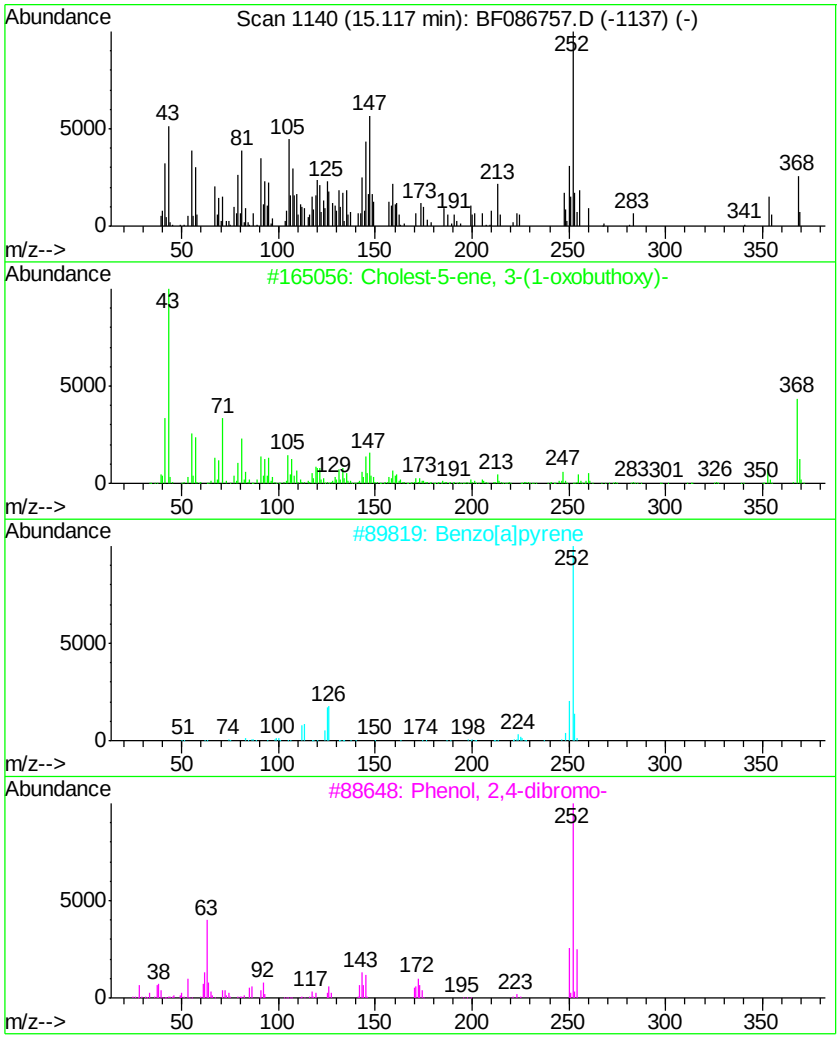
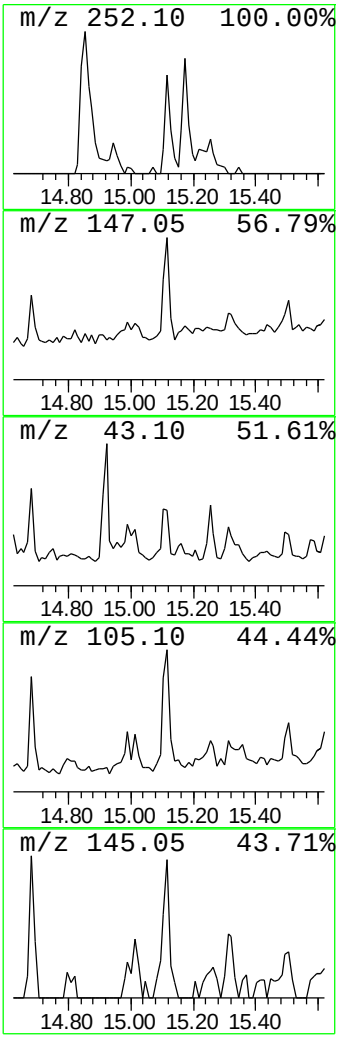
Peak Number 10 unknown15.12 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	4.76 ng	110785	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-ene, 3-(1-oxobuthoxy)-	456	C31H52O2	137036-79-4	43
2	Benzo[a]pyrene	252	C20H12	000050-32-8	35
3	Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	30
4	Perylene	252	C20H12	000198-55-0	25
5	1-Amino-4-(phenylthio)isoquinoline	252	C15H12N2S	019653-19-1	25





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Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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

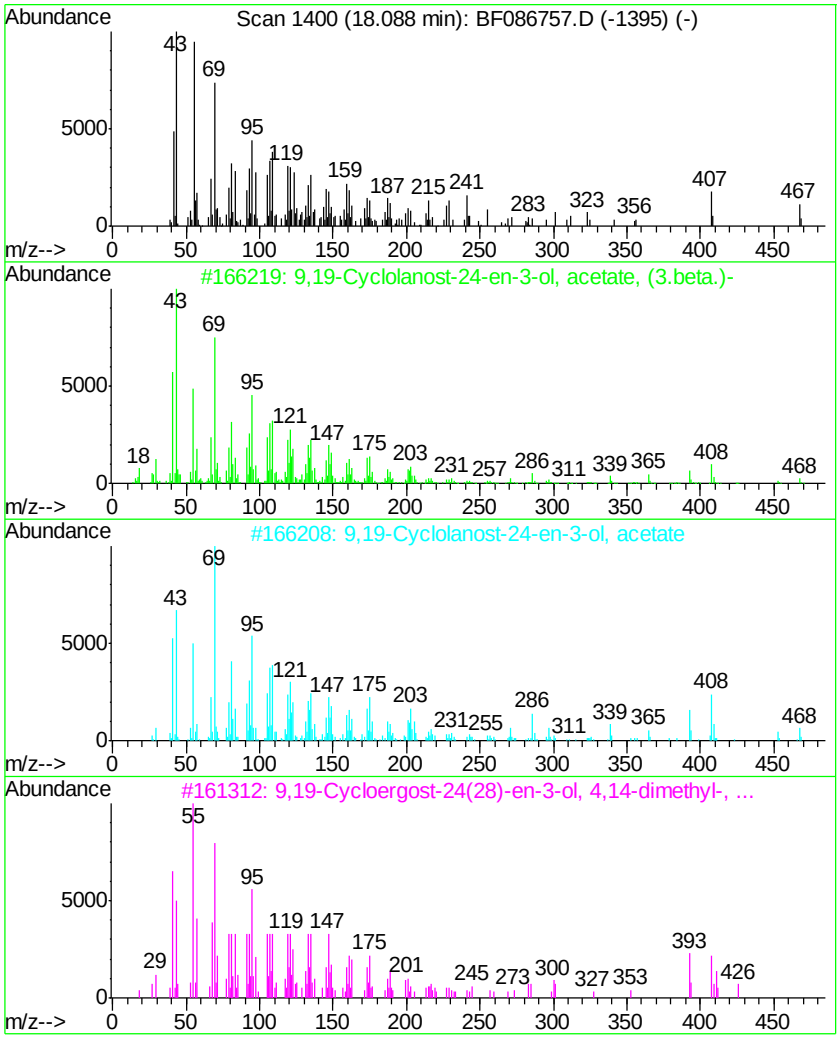
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

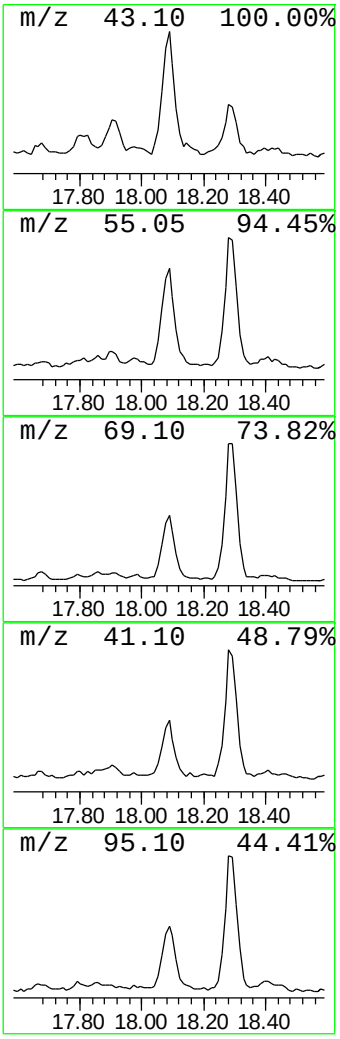
****

Peak Number 11 9,19-Cyclolanost-24-en-3-ol... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.09	18.81 ng	438203	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,19-Cyclolanost-24-en-3-ol, ace...	468	C32H52O2	001259-10-5	76
2	9,19-Cyclolanost-24-en-3-ol, ace...	468	C32H52O2	124094-10-6	50
3	9,19-Cycloergost-24(28)-en-3-ol,...	426	C30H50O	000469-39-6	45
4	9,19-Cycloergost-24(28)-en-3-ol,...	468	C32H52O2	010376-42-8	38
5	Silane, (9,19-cyclo-9.beta.-lano...	498	C33H58OSi	017608-55-8	37





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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

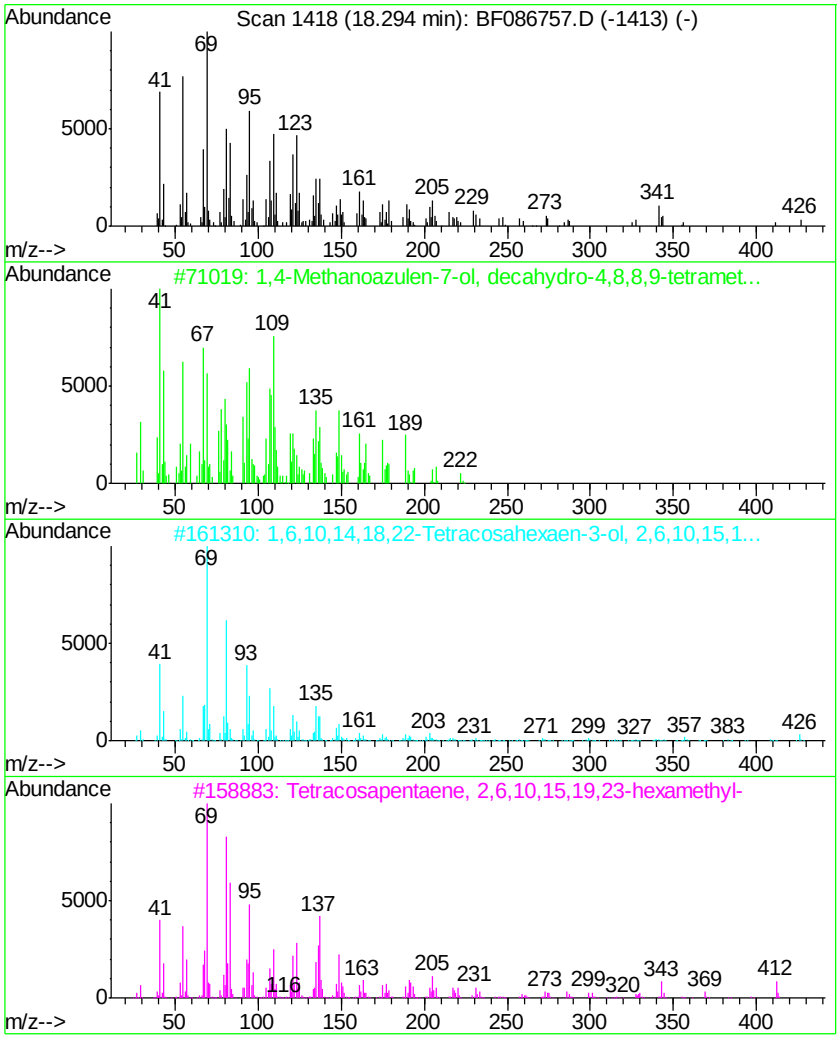
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

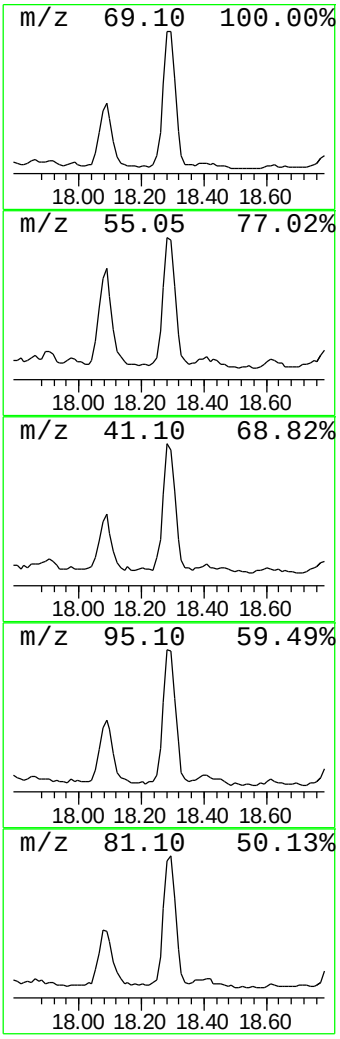
****

Peak Number 12 1,4-Methanoazulen-7-ol, dec... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	25.42 ng	592184	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Methanoazulen-7-ol, decahydr...	222	C15H26O	018319-27-2	56
2	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	054159-46-5	50
3	Tetracosapentaene, 2,6,10,15,19,...	412	C30H52	026266-08-0	47
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	42
5	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086757.D
Acq On : 7 May 2016 7:05
Operator : UM/SJ
Sample : H2720-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS1

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...	4.91	13.4	ng	423047	1	6.70	1267640	40.0
unknown6.48	6.48	171.2	ng	5426780	1	6.70	1267640	40.0
Hexadecane	10.18	6.2	ng	271127	3	9.73	1753810	40.0
Eicosane	10.65	9.1	ng	387410	4	11.22	1710820	40.0
n-Hexadecanoic acid	11.76	10.8	ng	462432	4	11.22	1710820	40.0
Octadecanoic acid	12.54	11.8	ng	381724	5	13.85	1289770	40.0
1-Docosene	13.71	7.1	ng	229102	5	13.85	1289770	40.0
Cyclotetracosane	14.35	4.4	ng	142815	5	13.85	1289770	40.0
unknown15.12	15.12	4.8	ng	110785	6	15.22	931666	40.0
9,19-Cyclolanost-...	18.09	18.8	ng	438203	6	15.22	931666	40.0
1,4-Methanoazulen...	18.29	25.4	ng	592184	6	15.22	931666	40.0