LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

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-BF060716.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	1.690	8	9	18	rVV	328042	571706	21.17%	1.791%
2	1.815	18	20	32	rVV	1471139	2452308	90.82%	7.680%
3	1.976	32	34	37	rVB	79700	101544	3.76%	0.318%
4	4.924	290	292	300	rBV	129815	220595	8.17%	0.691%
5	5.336	326	328	331	rBV	1825152	2698264	99.93%	8.451%
6	6.387	417	420	423	rBV	1965788	2365798	87.61%	7.409%
7	6.513	428	431	433	rVV	2439713	2567848	95.10%	8.042%
8	6.582	435	437	439	rBV	85361	72613	2.69%	0.227%
9	6.742	449	451	453	rBV	811401	674079	24.96%	2.111%
10	6.902	462	465	467	rBV	2262407	2249032	83.29%	7.044%
11	7.313	498	501	503	rBV	1683815	1786924	66.18%	5.596%
12	7.439	510	512	517	rBV	32193	59148	2.19%	0.185%
13	8.033	561	564	566	rBV	747685	850546	31.50%	2.664%
14	8.570	608	611	613	rBV	49140	48263	1.79%	0.151%
15	9.108	655	658	661	rBV	2482497	2700242	100.00%	8.457%
16	9.508	690	693	695	rVB	617693	567720	21.02%	1.778%
17	9.645	702	705	707	rBV	37932	39119	1.45%	0.123%
18	9.725	710	712	714	rBV	70393	59668	2.21%	0.187%
19	9.782	714	717	719	rBV	992483	898693	33.28%	2.815%
20	10.193	748	753	754	rBV	28117	34885	1.29%	0.109%
21	10.216	754	755	757	rVB	67932	77317	2.86%	0.242%
22	10.433	771	774	776	rBV	30725	50126	1.86%	0.157%
23	10.571	783	786	788	rBV	1436309	1535914	56.88%	4.810%
24	10.696	795	797	801	rBV	82178	122939	4.55%	0.385%
25	11.142	832	836	837	rBV	54224	61589	2.28%	0.193%
26	11.256	844	846	850	rVB	735621	822046	30.44%	2.575%
27	11.336	850	853	855	rBV	60705	67089	2.48%	0.210%
28	11.496	864	867	871	rBV3	55896	83278	3.08%	0.261%
29	11.794	891	893	895	rVB2	27686	38271	1.42%	0.120%
30	11.874	898	900	904	rVB2	45602	86157	3.19%	0.270%
31	11.977	904	909	913	rBV3	25827	61970	2.29%	0.194%
32	12.308	935	938	940	rBV	51207	60097	2.23%	0.188%
33	12.365	940	943	944	rVV2	31155	57122	2.12%	0.179%
34	12.399	944	946	950	rVB	27969	38802	1.44%	0.122%

LSC Area Percent Report

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Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.468	950	952	954	rBV	474475	401160	14.86%	1.256%
36	12.697	969	972	974	rBV	409742	571030	21.15%	1.788%
37	12.754	976	977	979	rVB	63432	50249	1.86%	0.157%
38	12.845	982	985	988	rVB	1885082	1925181	71.30%	6.029%
39	12.914	988	991	995	rVB3	45341	73899	2.74%	0.231%
40	13.028	997	1001	1002	rVB	49718	105889	3.92%	0.332%
41	13.085	1002	1006	1008	rBV3	42138	62313	2.31%	0.195%
42	13.131	1008	1010	1012	rBV	59293	74760	2.77%	0.234%
43	13.222	1013	1018	1019	rVB2	35740	45800	1.70%	0.143%
44	13.245	1019	1020	1023	rBV2	25597	36609	1.36%	0.115%
45	13.382	1030	1032	1034	rBV	112245	114821	4.25%	0.360%
46	13.428	1034	1036	1039	rVB3	36129	67069	2.48%	0.210%
47	13.531	1044	1045	1049	rVV	64164	71259	2.64%	0.223%
48	13.645	1052	1055	1056	rVV2	42132	75232	2.79%	0.236%
49	13.691	1058	1059	1062	rVV2	40490	52793	1.96%	0.165%
50	13.748	1062	1064	1068	rVV3	83192	149698	5.54%	0.469%
51	13.885	1072	1076	1083	rBV3	621814	1196864	44.32%	3.748%
52	14.000	1083	1086	1087	rBV2	24553	38095	1.41%	0.119%
53	14.068	1090	1092	1094	rVB2	42700	48624	1.80%	0.152%
54	14.274	1108	1110	1112	rVB	43019	59465	2.20%	0.186%
55	14.308	1112	1113	1115	rBV2	27006	36871	1.37%	0.115%
56	14.377	1115	1119	1120	rBV3	55760	76087	2.82%	0.238%
57	14.662	1142	1144	1148	rVB2	35625	77926	2.89%	0.244%
58	14.742	1148	1151	1155	rBV3	31266	82360	3.05%	0.258%
59	14.800	1155	1156	1159	rVB3	21986	35369	1.31%	0.111%
60	14.903	1162	1165	1170	rBV	239917	478872	17.73%	1.500%
61	14.983	1170	1172	1175	rBV3	95464	171897	6.37%	0.538%
62	15.177	1187	1189	1192	rVB	136191	167905	6.22%	0.526%
63	15.234	1192	1194	1196	rBV	163085	189643	7.02%	0.594%
64	15.291	1196	1199	1201	rBV	540563	657847	24.36%	2.060%
65	15.508	1215	1218	1220	rVB2	26536	39283	1.45%	0.123%
66	15.714	1233	1236	1239	rBV	85079	132703	4.91%	0.416%
67	16.320	1284	1289	1295	rVB7	11638	40164	1.49%	0.126%
68	16.617	1312	1315	1320	rBV2	51515	115019	4.26%	0.360%
69	16.697	1320	1322	1326	rVB	20634	38911	1.44%	0.122%
70	16.788	1326	1330	1332	rBV2	11190	32854	1.22%	0.103%
71	17.017	1347	1350	1356	rVB	36824	80978	3.00%	0.254%

LSC Area Percent Report

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Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	18.046	1436	1440	1448	rBV6	10484	32636	1.21%	0.102%
73	19.063	1524	1529	1535	rVB2	10294	39915	1.48%	0.125%

Sum of corrected areas: 31929762

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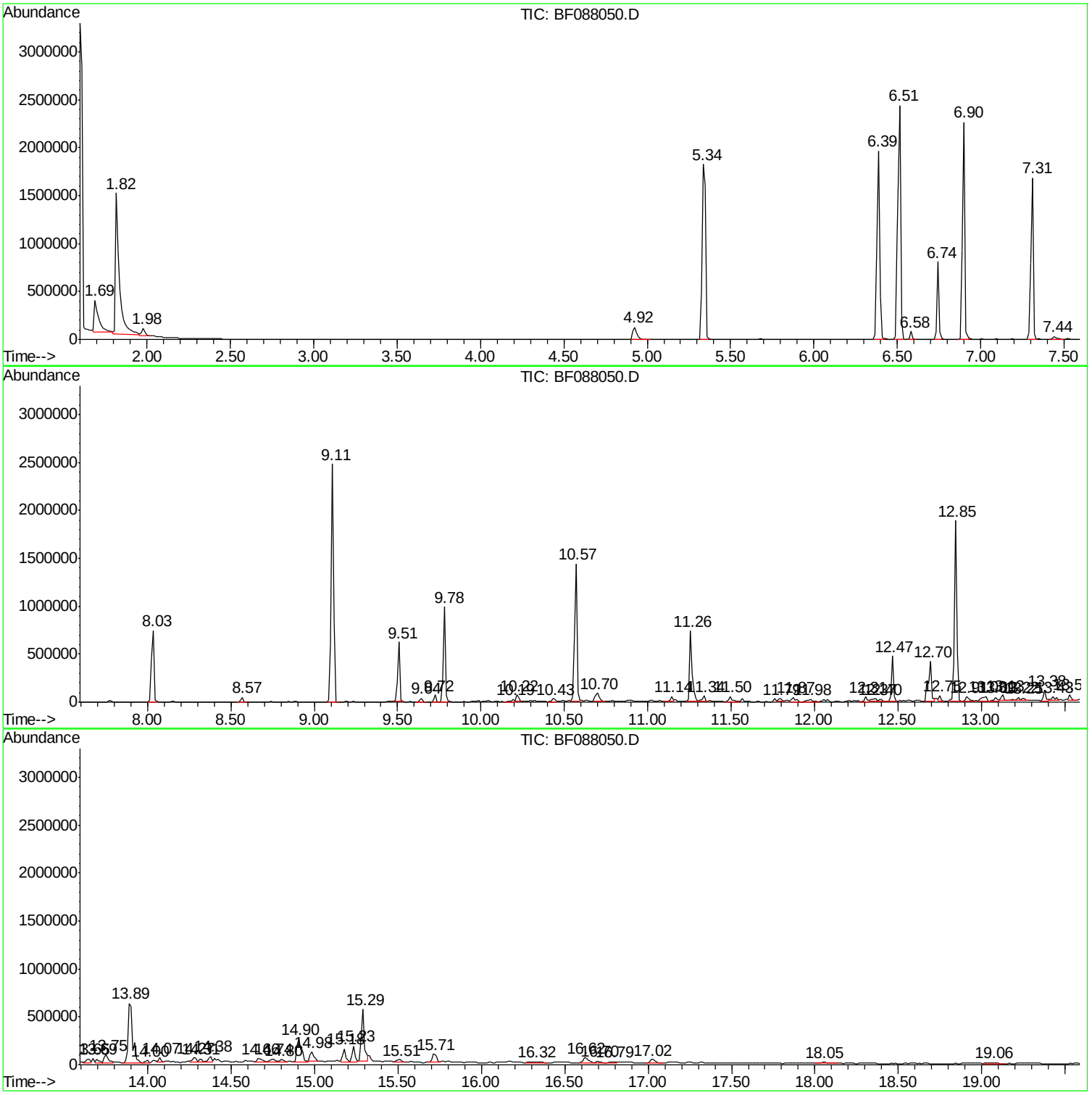
Instrument :
BNA_F
ClientSampleId :
STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
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Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

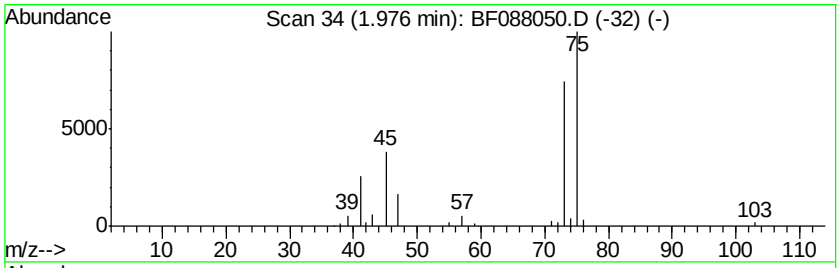
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

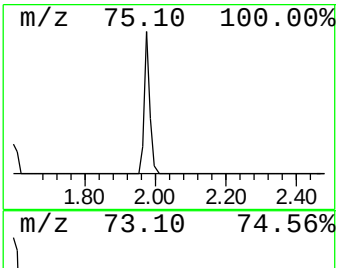
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.98	3.01 ng	101544	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
3	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

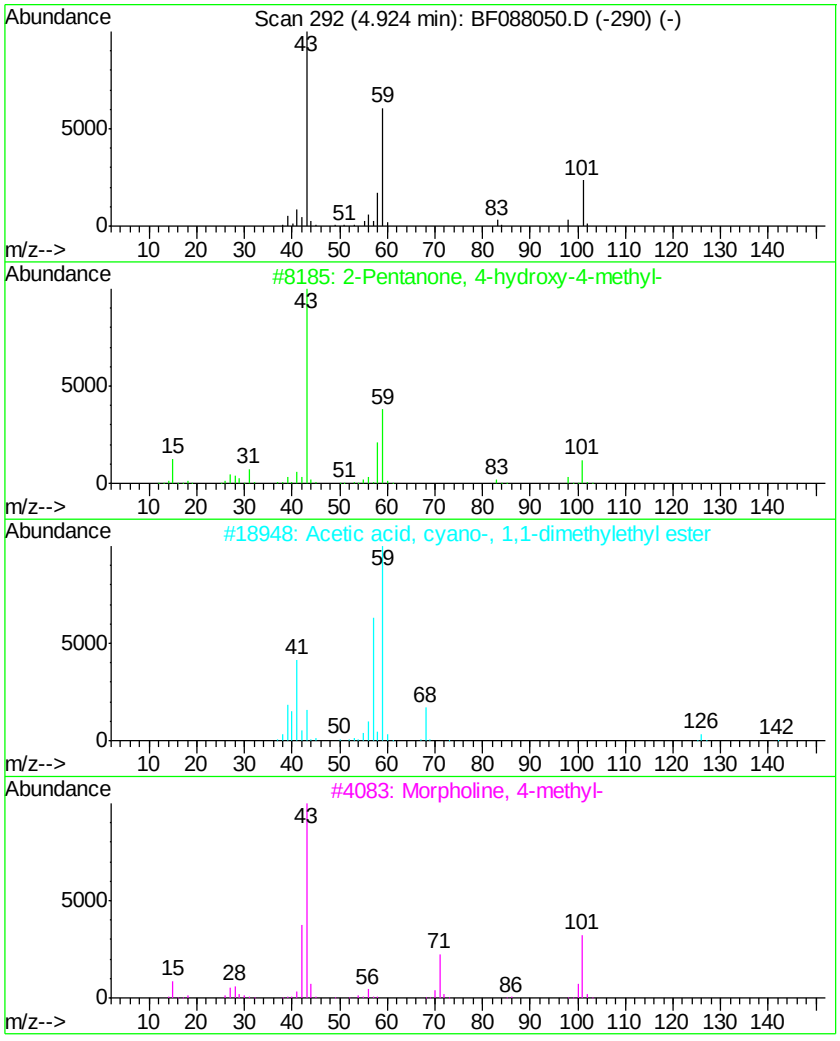
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

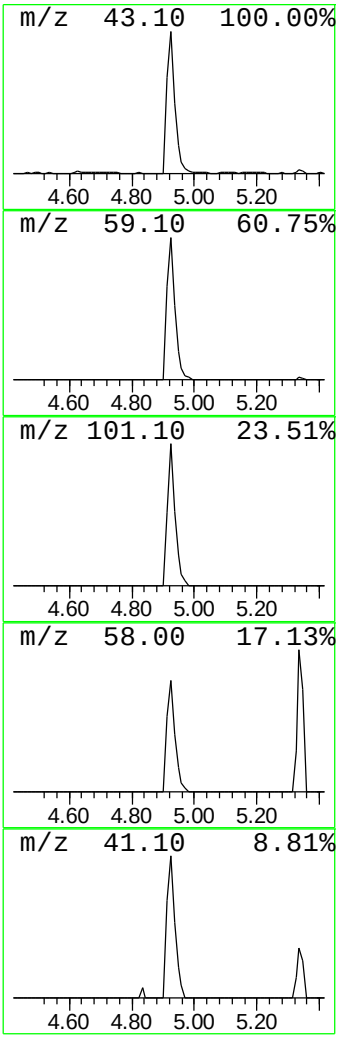
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	6.55 ng	220595	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

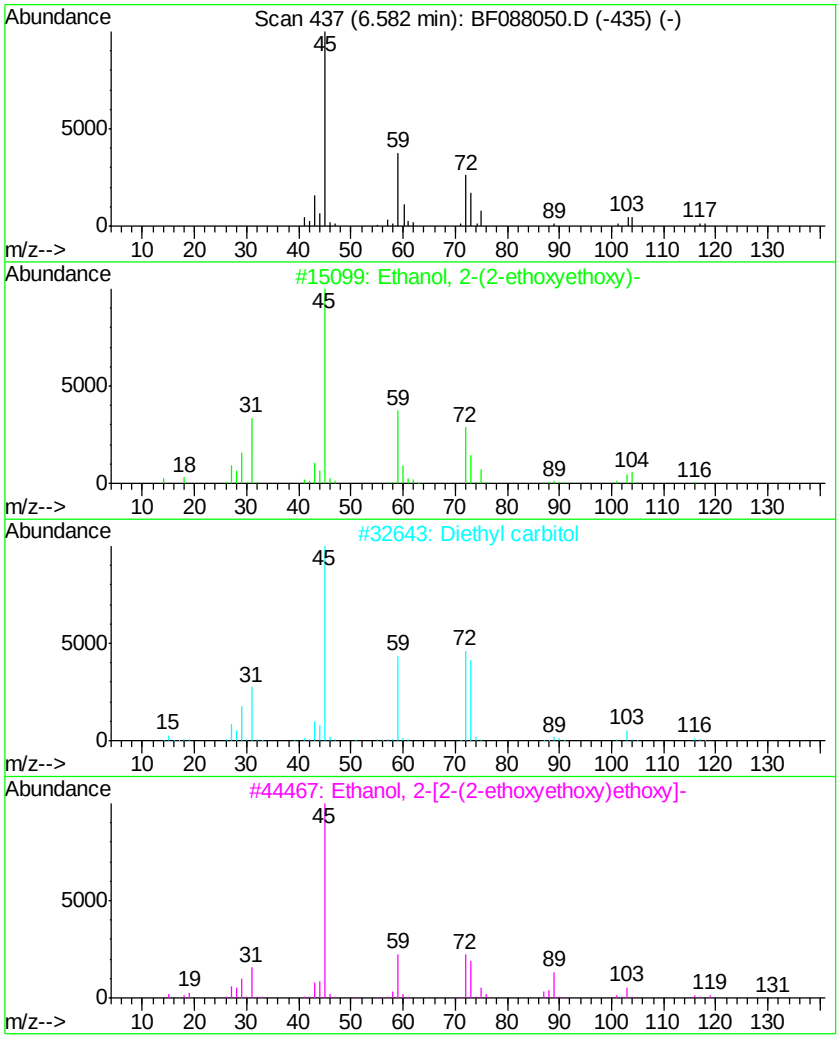
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

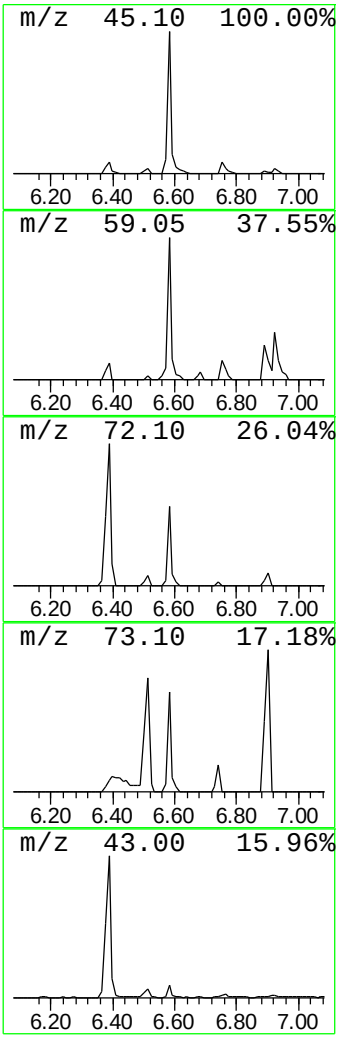
****

Peak Number 6 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	2.15 ng	72613	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	72
4	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5	Trimethylene glycol monomethyl e...	90	C4H10O2	001589-49-7	42





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
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Misc :
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Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

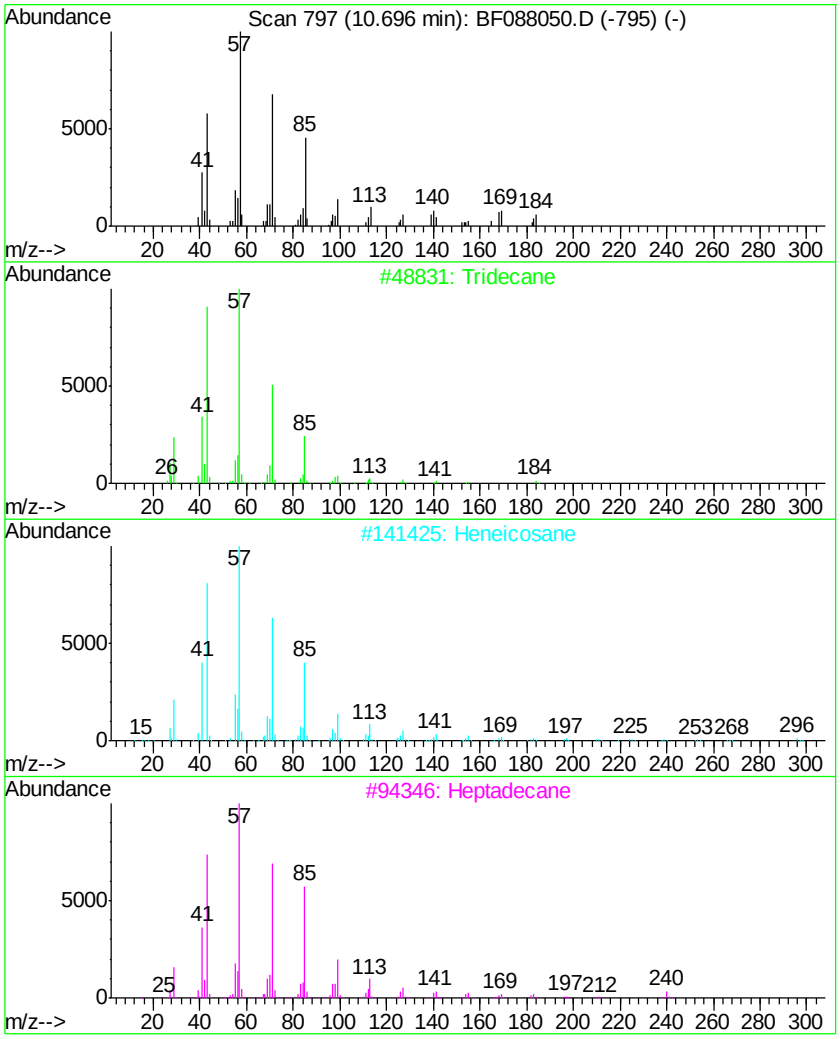
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

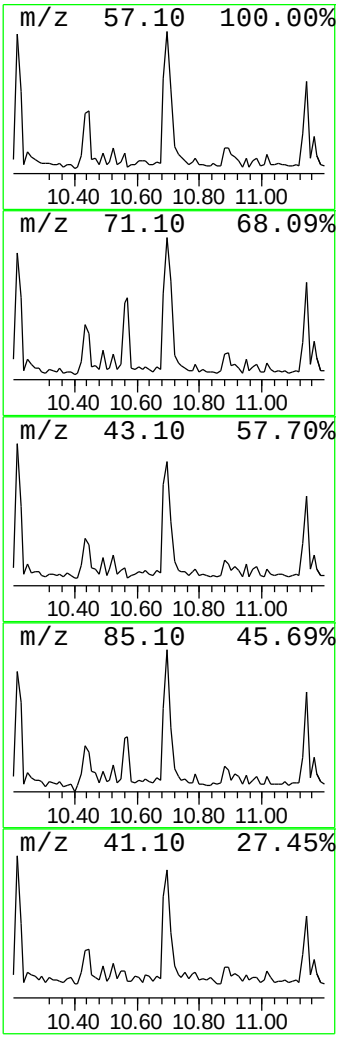
****

Peak Number 8 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.99 ng	122939	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Heptadecane	240	C17H36	000629-78-7	87
4	Octadecane	254	C18H38	000593-45-3	86
5	Eicosane	282	C20H42	000112-95-8	86





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Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

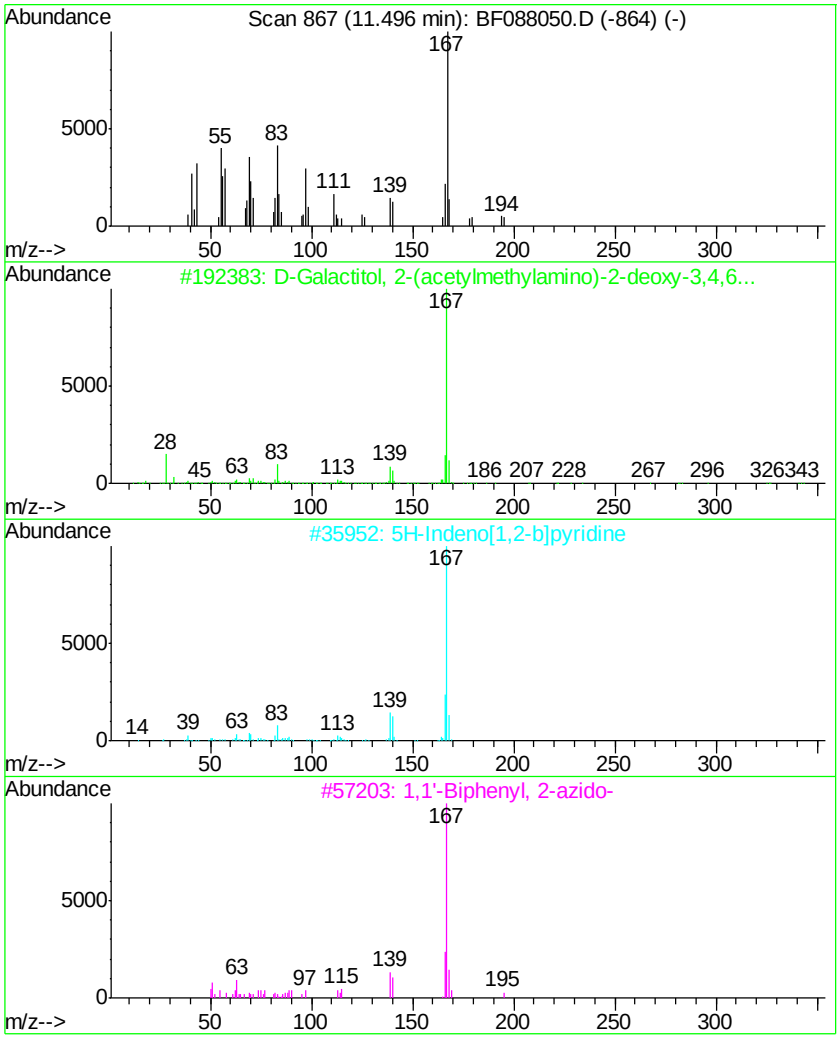
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

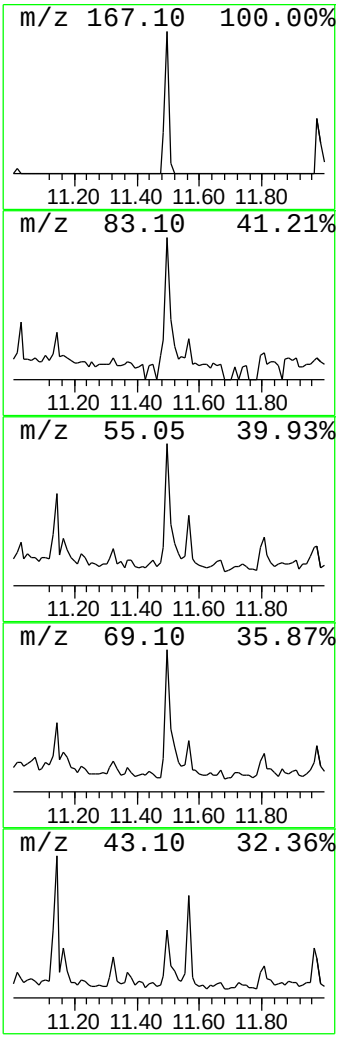
****

Peak Number 9 D-Galactitol, 2-(acetylmeth... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	2.03 ng	83278	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Galactitol, 2-(acetylmethylami...	363	C16H29NO8	074410-42-7	53
2	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	49
3	1,1'-Biphenyl, 2-azido-	195	C12H9N3	007599-23-7	49
4	Carbazole	167	C12H9N	000086-74-8	49
5	Thiazolo[3,2-a]pyridinium, 2,3-d...	167	C8H9NOS	023003-43-2	49





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Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

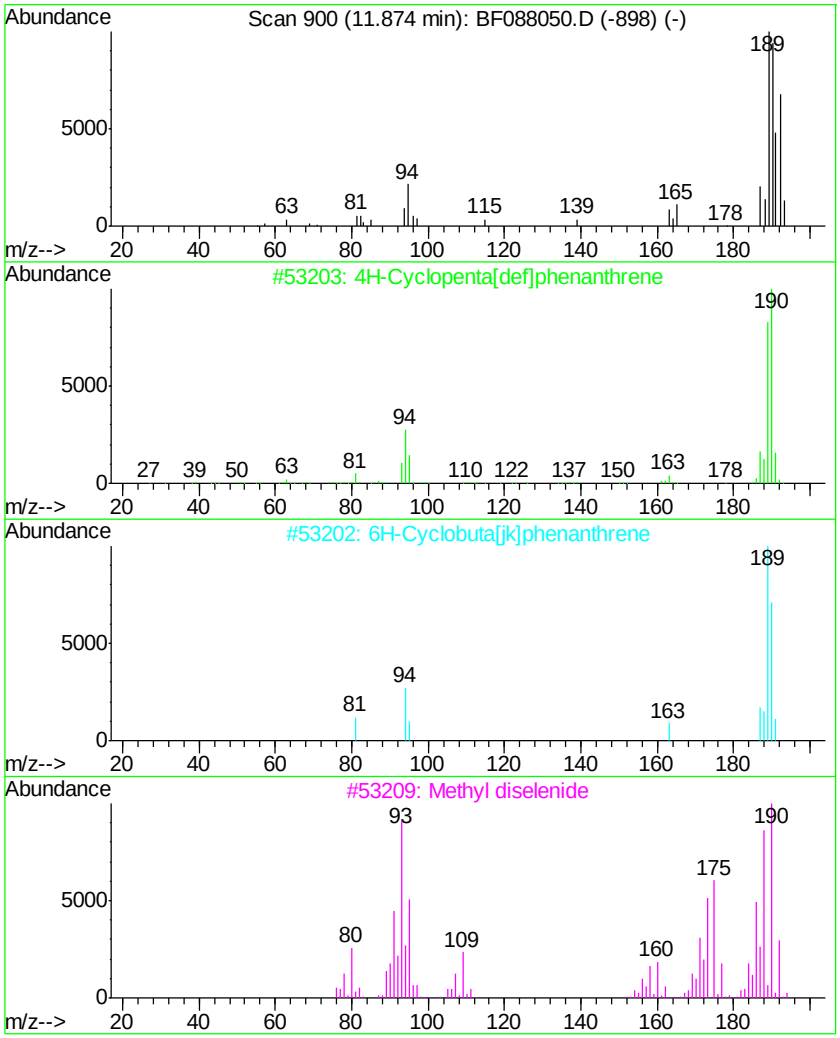
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

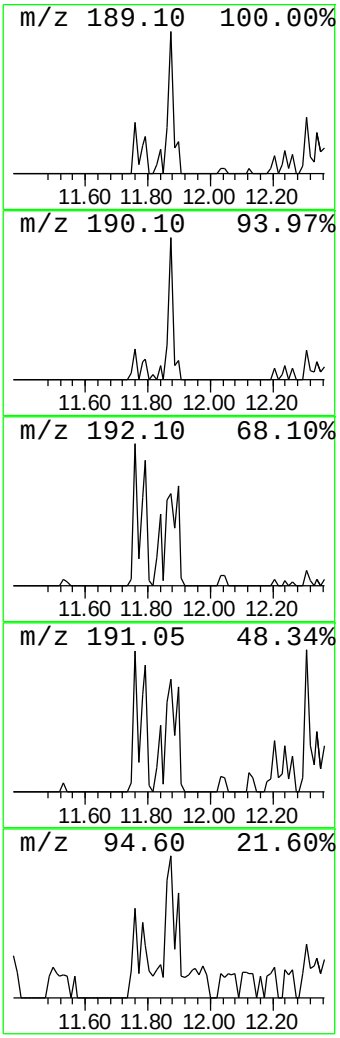
****

Peak Number 10 4H-Cyclopenta[def]phenanthrene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.10 ng	86157	Phenanthrene-d10	11.26

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	58
3	Methyl diselenide	190	C2H6Se2	007101-31-7	41
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	30
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

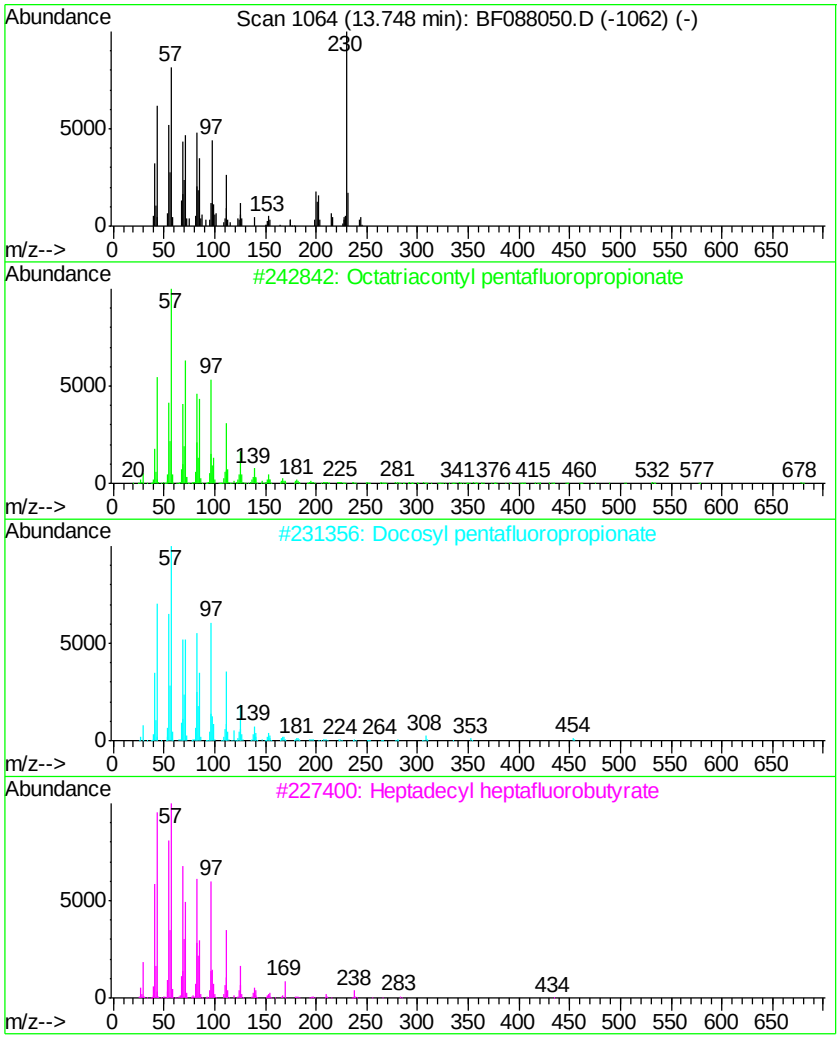
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

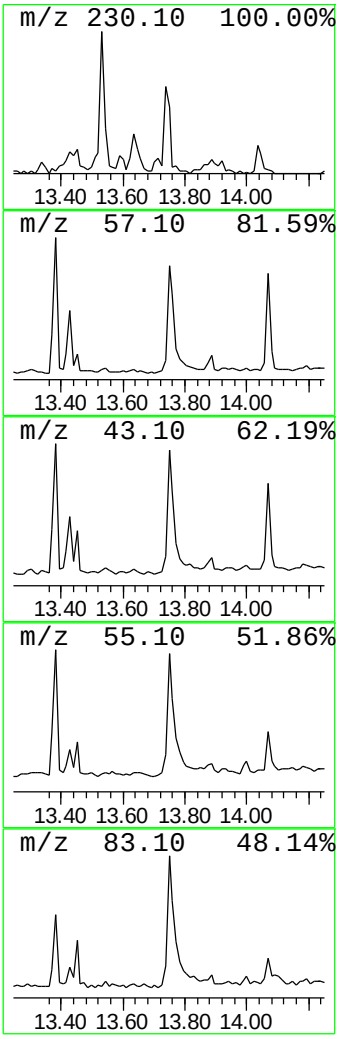
****

Peak Number 11 Octatriacontyl pentafluorop... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	2.50 ng	149698	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	60
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	60
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	60
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	60
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	60





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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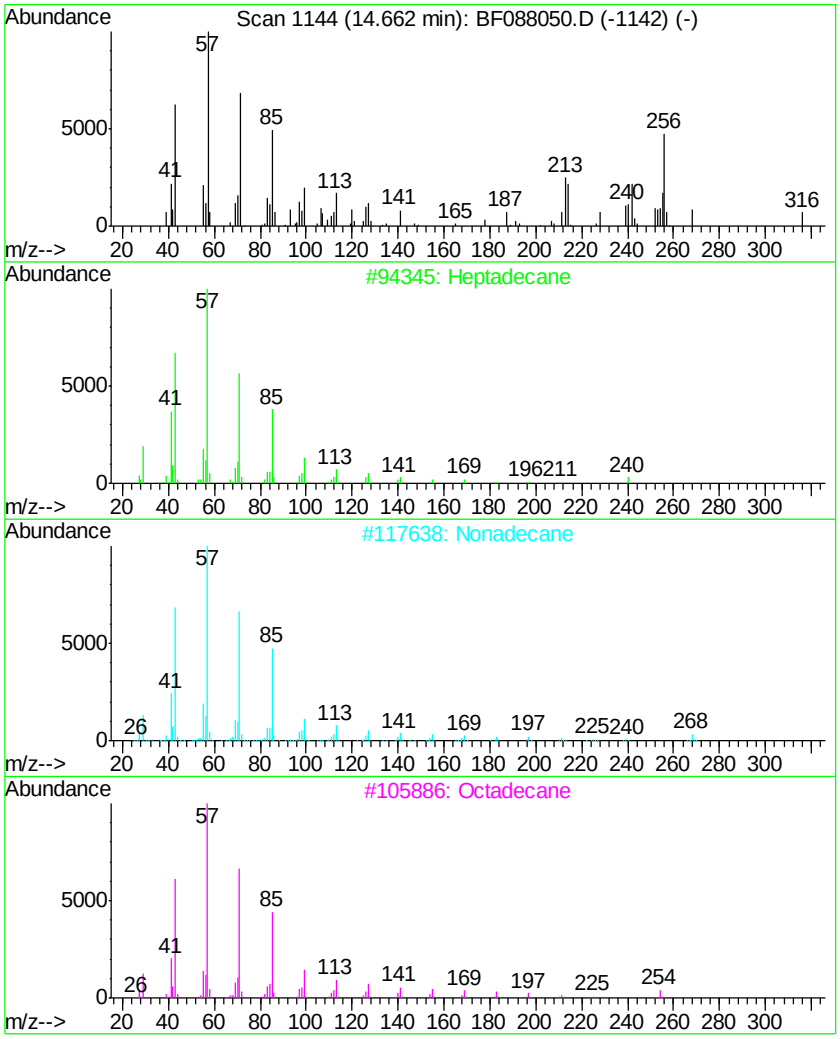
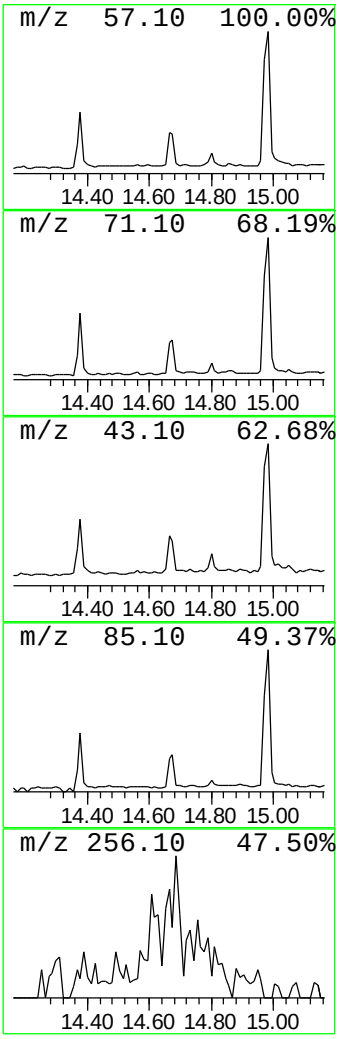
Peak Number 12 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.37 ng	77926	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Nonadecane	268	C19H40	000629-92-5	49
3	Octadecane	254	C18H38	000593-45-3	46
4	Octacosane	394	C28H58	000630-02-4	38
5	Pentacosane	352	C25H52	000629-99-2	38





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Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
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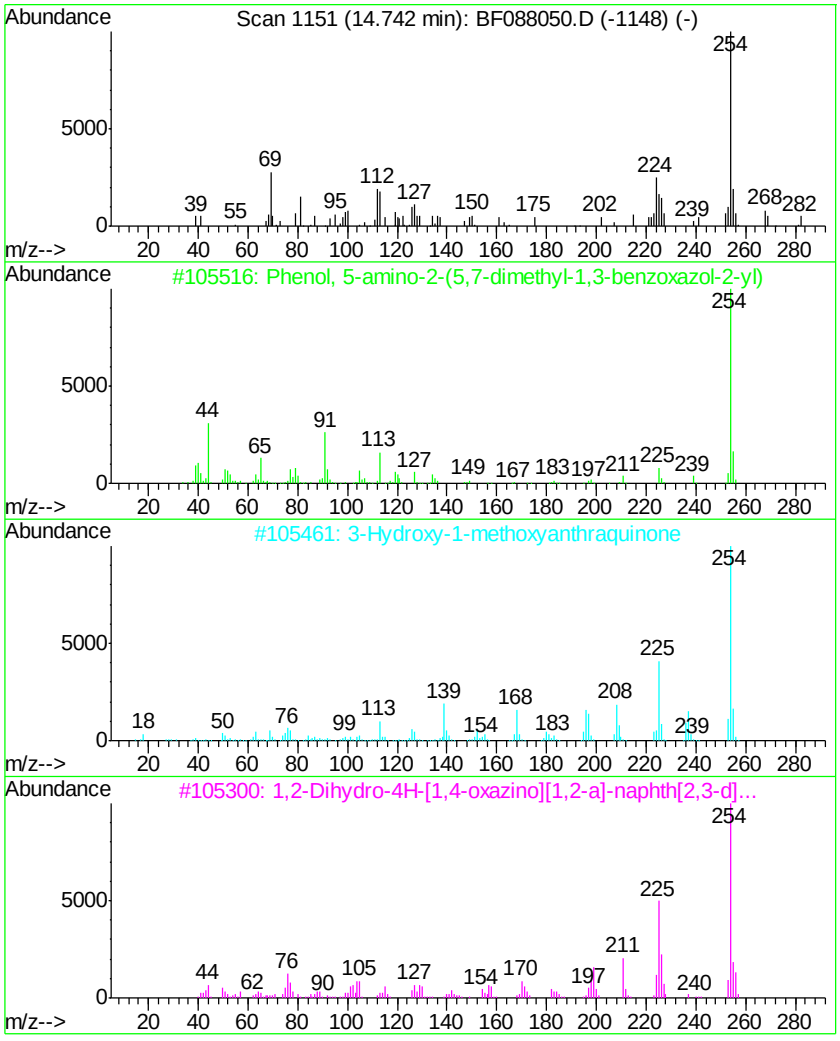
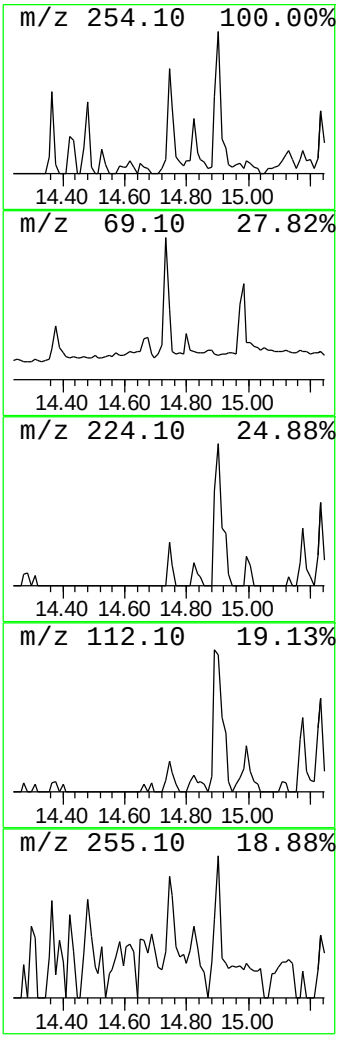
Peak Number 13 Phenol, 5-amino-2-(5,7-dime... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.50 ng	82360	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 5-amino-2-(5,7-dimethyl-...	254	C15H14N2O2	1000338-06-4	58
2	3-Hydroxy-1-methoxyanthraquinone	254	C15H10O4	028504-24-7	50
3	1,2-Dihydro-4H-[1,4-oxazino][1,2...	254	C14H10N2O3	038066-84-1	50
4	3-(2-Furan-2-yl-2-oxo-ethylidene...	254	C14H10N2O3	1000297-32-1	50
5	Chrysin	254	C15H10O4	000480-40-0	50





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Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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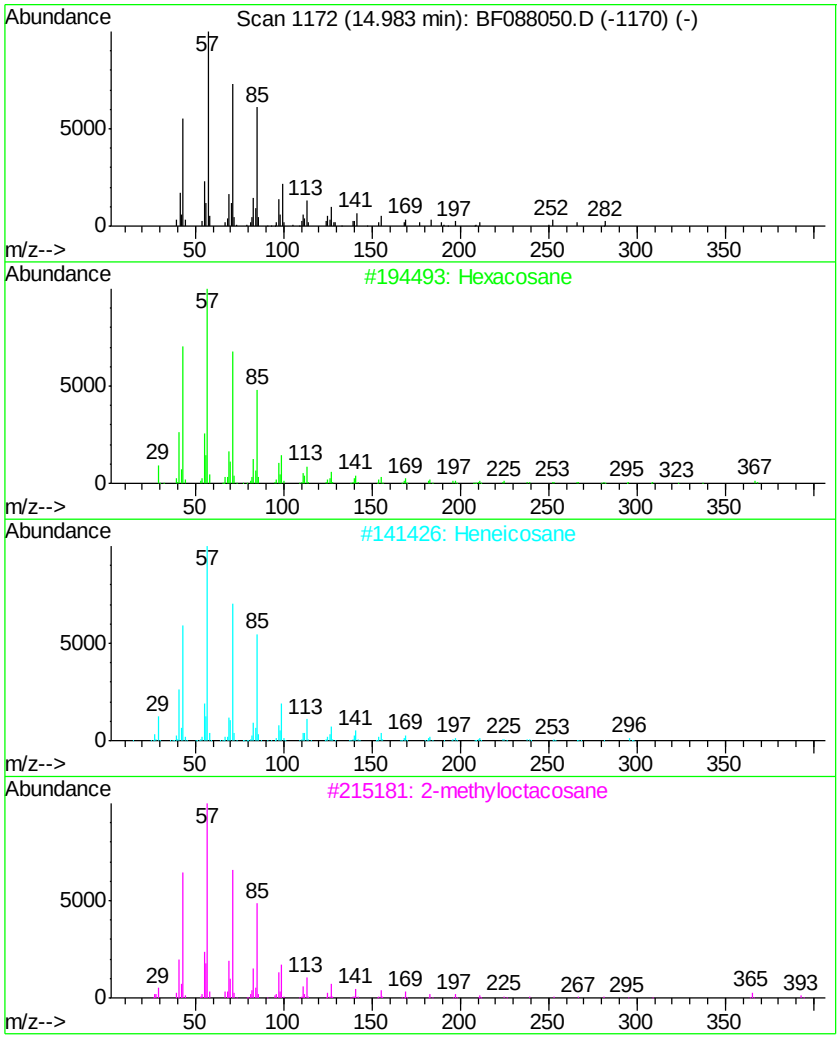
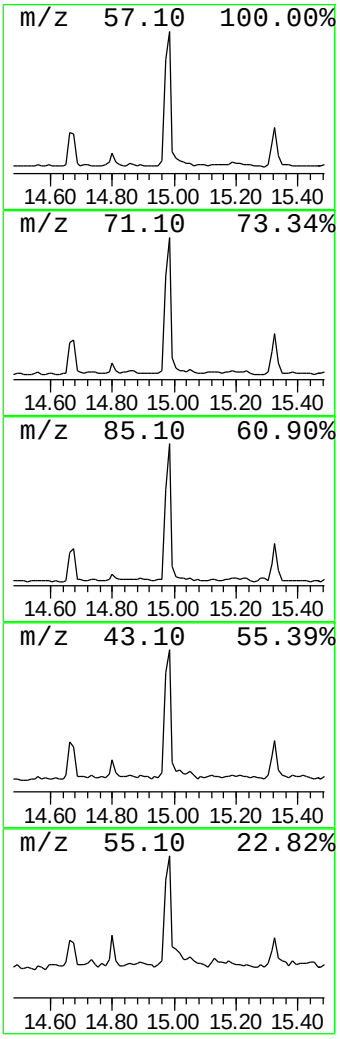
Peak Number 14 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	5.23 ng	171897	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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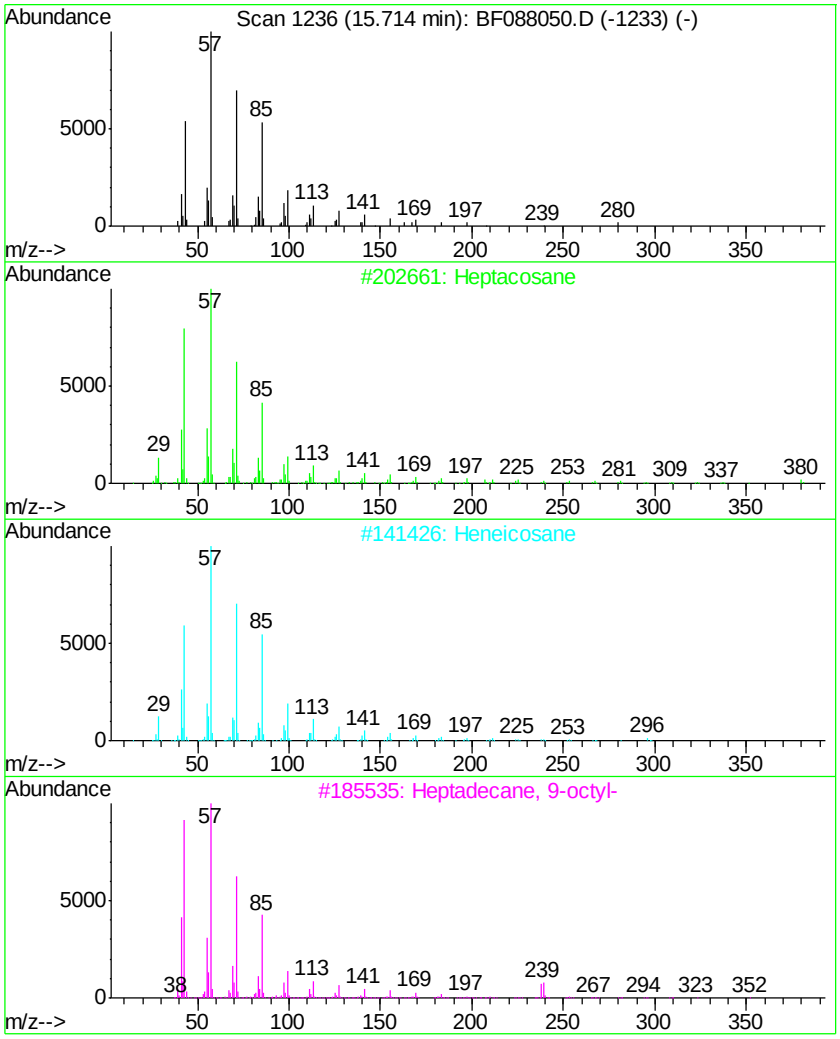
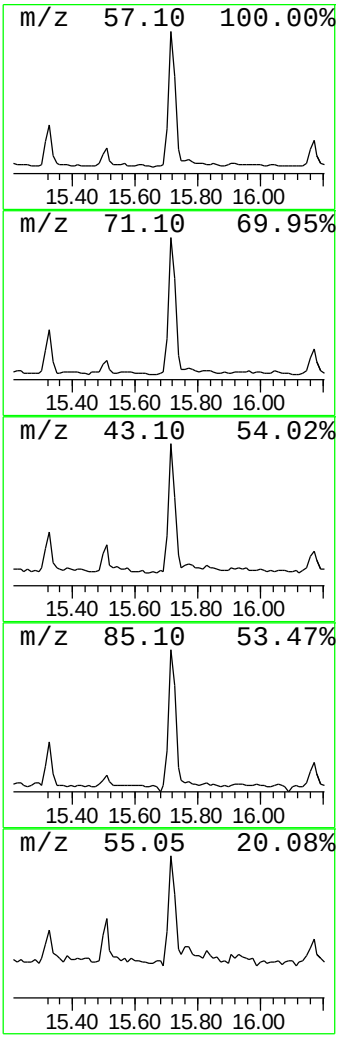
Peak Number 16 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	4.03 ng	132703	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061516\
Data File : BF088050.D
Acq On : 15 Jun 2016 23:03
Operator : UM/SJ
Sample : H3471-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1045-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	1.98	3.0	ng	101544	1	6.74	674079	20.0
2-Pentanone, 4-hy...	4.92	6.5	ng	220595	1	6.74	674079	20.0
Ethanol, 2-(2-eth...	6.58	2.1	ng	72613	1	6.74	674079	20.0
Tridecane	10.70	3.0	ng	122939	4	11.26	822046	20.0
D-Galactitol, 2-(...	11.50	2.0	ng	83278	4	11.26	822046	20.0
4H-Cyclopenta[def...	11.87	2.1	ng	86157	4	11.26	822046	20.0
Octatriacontyl pe...	13.75	2.5	ng	149698	5	13.90	1196860	20.0
Heptadecane	14.66	2.4	ng	77926	6	15.29	657847	20.0
Phenol, 5-amino-2...	14.74	2.5	ng	82360	6	15.29	657847	20.0
Hexacosane	14.98	5.2	ng	171897	6	15.29	657847	20.0
Heptacosane	15.71	4.0	ng	132703	6	15.29	657847	20.0