LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102115\
Data File : BF082431.D
Acq On : 22 Oct 2015 5:06
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

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-BF101015.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	4.937	242	245	255	rVB	751185	1114368	58.46%	5.544%
2	5.360	280	282	285	rBV	1168687	1636186	85.84%	8.140%
3	5.772	316	318	320	rBV	14711	21051	1.10%	0.105%
4	6.412	372	374	377	rBV	1137720	1615966	84.78%	8.039%
5	6.537	383	385	388	rBV	1926984	1721104	90.29%	8.562%
6	6.766	403	405	408	rBV	643096	599364	31.44%	2.982%
7	6.926	417	419	421	rBV	1707994	1508439	79.13%	7.504%
8	7.337	453	455	458	rBV	907974	959874	50.36%	4.775%
9	8.057	516	518	520	rBV	947842	779397	40.89%	3.877%
10	9.143	610	613	615	rBV	1385351	1906177	100.00%	9.483%
11	9.532	645	647	650	rBV	324555	349689	18.35%	1.740%
12	9.818	669	672	674	rBV	739920	772254	40.51%	3.842%
13	10.241	708	709	711	rVB	33802	30361	1.59%	0.151%
14	10.606	738	741	743	rBV	912680	925316	48.54%	4.603%
15	10.721	749	751	754	rBV	44517	54533	2.86%	0.271%
16	11.166	788	790	791	rBV	38102	32342	1.70%	0.161%
17	11.304	800	802	803	rBV	623876	647374	33.96%	3.221%
18	11.326	803	804	806	rVV	61916	57432	3.01%	0.286%
19	11.361	806	807	810	rVB2	11257	19453	1.02%	0.097%
20	11.589	824	827	832	rVB2	20283	38023	1.99%	0.189%
21	11.795	844	845	847	rBV2	63475	74565	3.91%	0.371%
22	11.829	847	848	851	rVV2	101527	135650	7.12%	0.675%
23	11.909	854	855	859	rVB2	16177	27046	1.42%	0.135%
24	12.515	905	908	910	rBV	122836	124040	6.51%	0.617%
25	12.744	925	928	930	rBV	107891	116410	6.11%	0.579%
26	12.858	934	938	939	rBV3	11521	20474	1.07%	0.102%
27	12.892	939	941	943	rBV	1454792	1411430	74.05%	7.022%
28	13.075	953	957	958	rBV	12697	24187	1.27%	0.120%
29	13.121	958	961	964	rVV4	10392	24241	1.27%	0.121%
30	13.178	964	966	970	rVB3	12247	26179	1.37%	0.130%
31	13.589	1000	1002	1004	rVB	23279	26924	1.41%	0.134%
32	13.704	1009	1012	1013	rBV3	10328	20293	1.06%	0.101%
33	13.749	1015	1016	1019	rVV2	9828	24033	1.26%	0.120%
34	13.807	1019	1021	1026	rVB	72572	136154	7.14%	0.677%

LSC Area Percent Report

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Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

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-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.955	1031	1034	1040	rVV	670850	826677	43.37%	4.113%
36	14.127	1047	1049	1052	rBV4	12970	34064	1.79%	0.169%
37	14.470	1075	1079	1085	rBV6	50109	180708	9.48%	0.899%
38	14.847	1110	1112	1113	rBV	28566	29827	1.56%	0.148%
39	14.915	1116	1118	1121	rVV	129948	156834	8.23%	0.780%
40	15.030	1125	1128	1132	rVV	61651	135397	7.10%	0.674%
41	15.098	1132	1134	1135	rBV	62146	68569	3.60%	0.341%
42	15.132	1135	1137	1142	rVB	141506	266032	13.96%	1.323%
43	15.315	1151	1153	1156	rVB	29733	38179	2.00%	0.190%
44	15.373	1156	1158	1161	rVB	49114	61054	3.20%	0.304%
45	15.430	1161	1163	1169	rBV	531621	720018	37.77%	3.582%
46	15.647	1180	1182	1184	rVB	37083	49923	2.62%	0.248%
47	15.864	1199	1201	1204	rBV	84800	149132	7.82%	0.742%
48	16.344	1241	1243	1244	rBV	17223	22875	1.20%	0.114%
49	16.824	1281	1285	1288	rBV	46464	114382	6.00%	0.569%
50	16.893	1288	1291	1294	rVV	32876	66853	3.51%	0.333%
51	16.950	1294	1296	1298	rVV3	20677	37655	1.98%	0.187%
52	17.236	1319	1321	1324	rVB	19913	37303	1.96%	0.186%
53	18.299	1411	1414	1421	rVB6	36763	125511	6.58%	0.624%

Sum of corrected areas: 20101322

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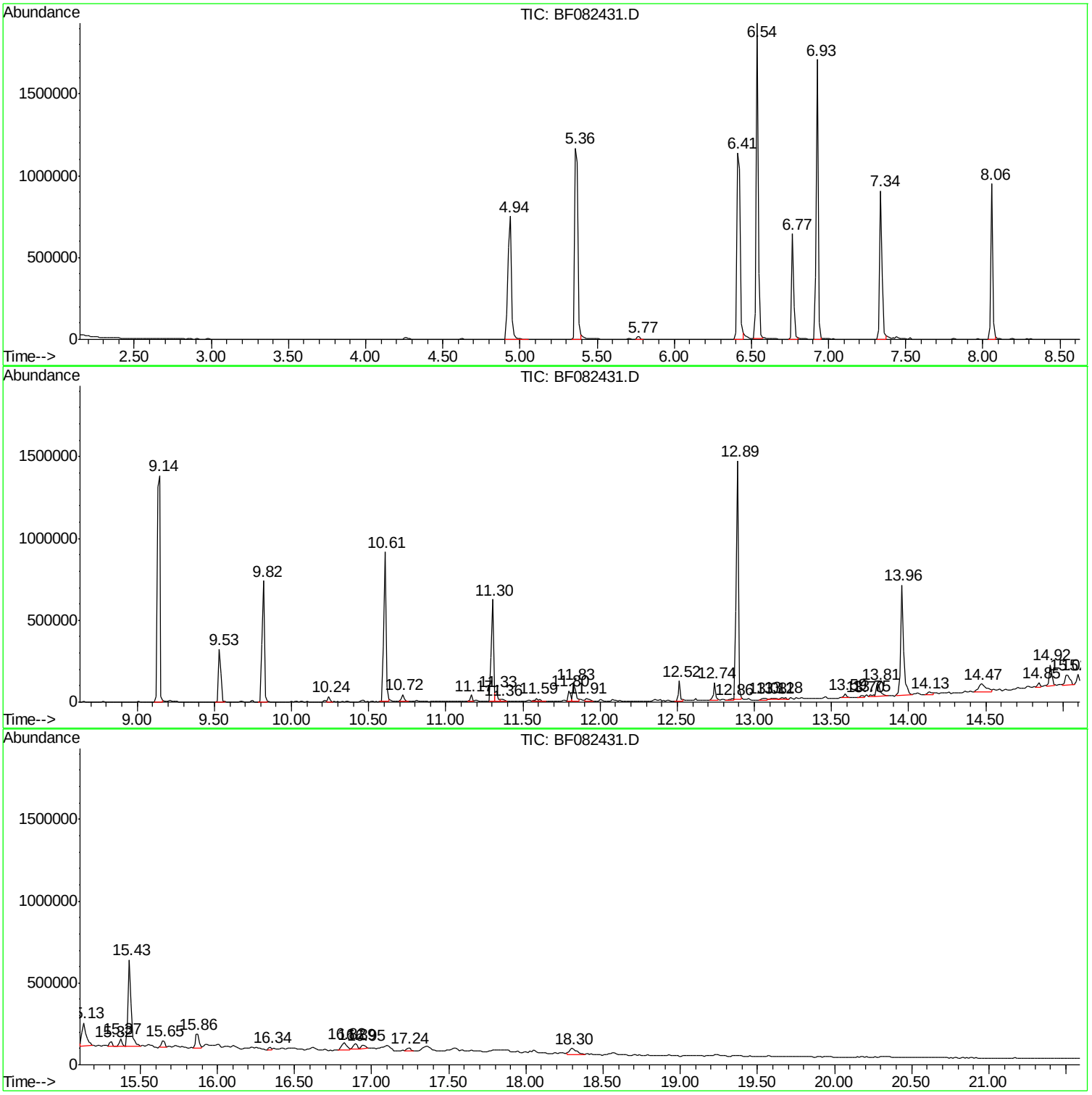
Instrument :
BNA_F
ClientSampleId :
BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF082431.D
Acq On : 22 Oct 2015 5:06
Operator : UM/IZ
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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST02.L
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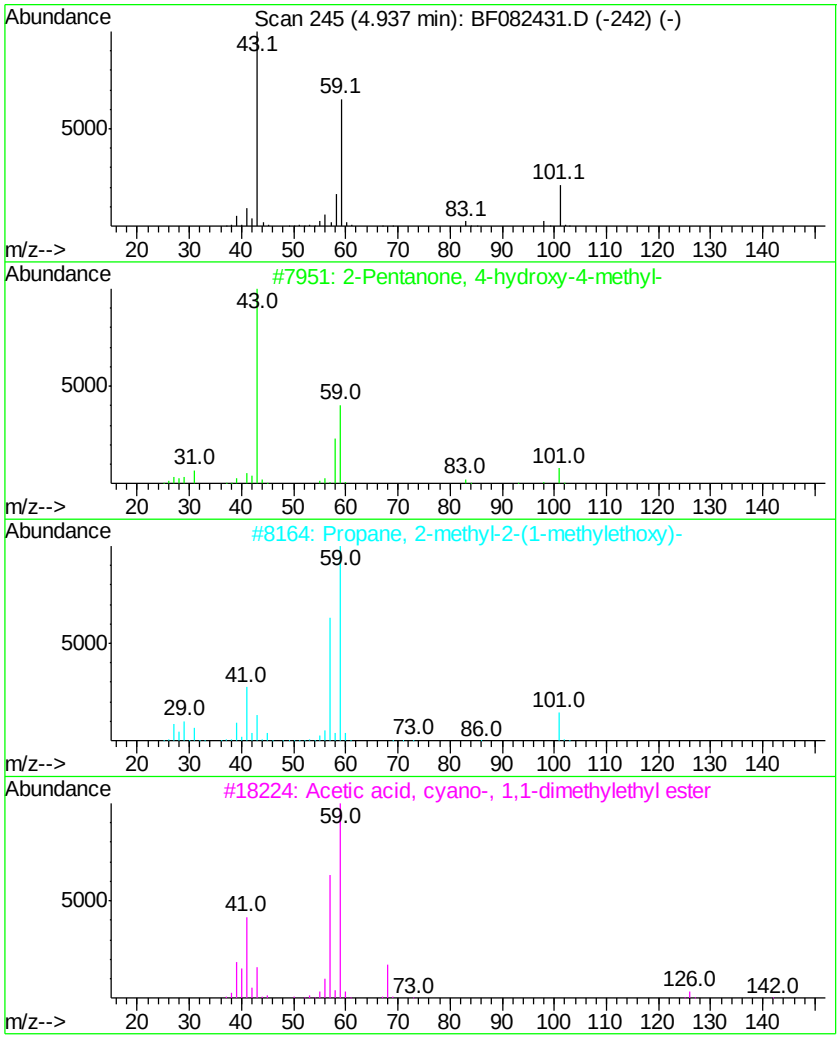
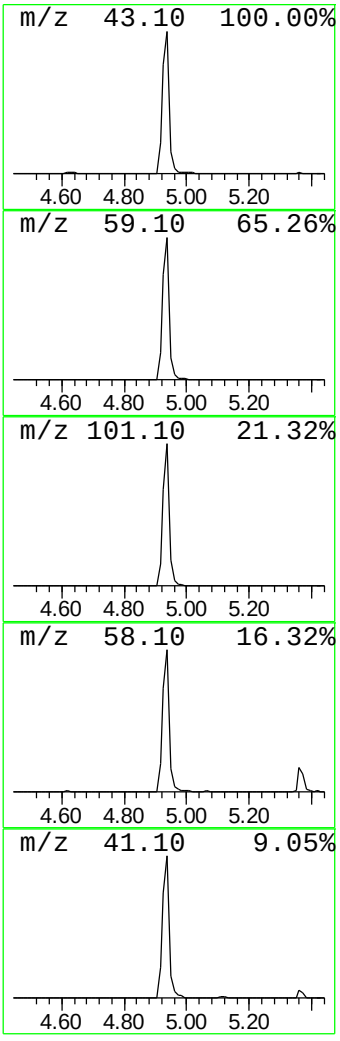
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	37.19 ng	1114370	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102115\
Data File : BF082431.D
Acq On : 22 Oct 2015 5:06
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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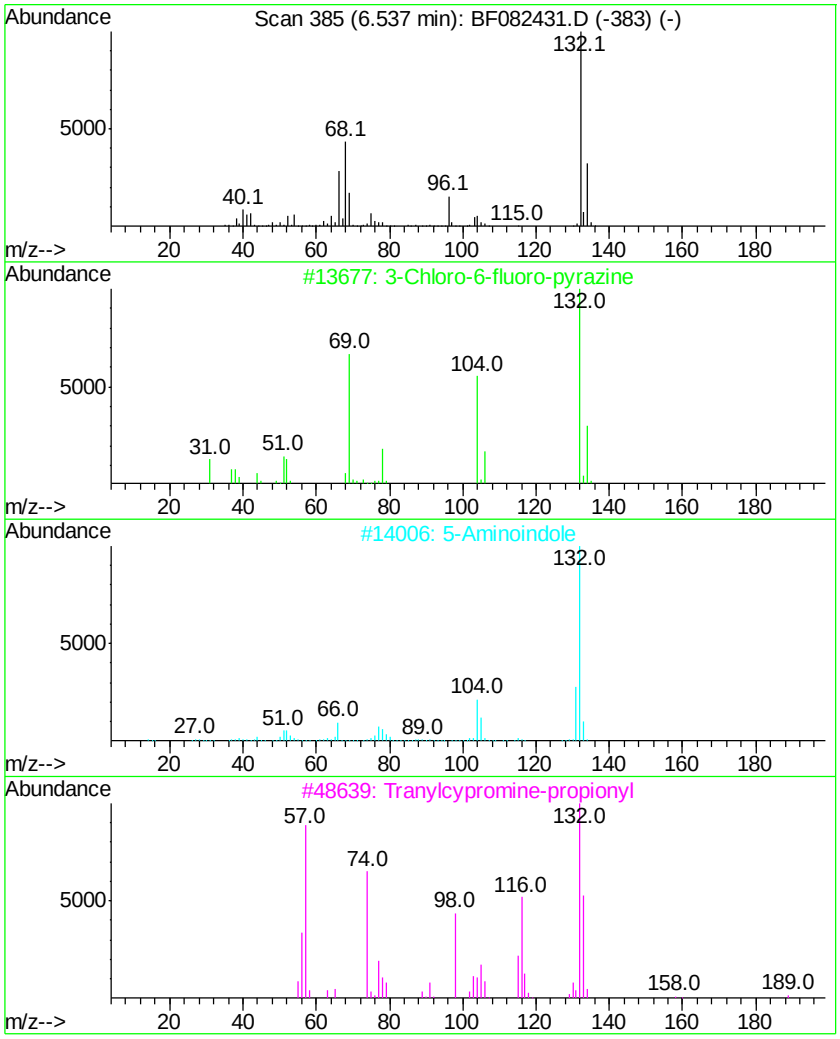
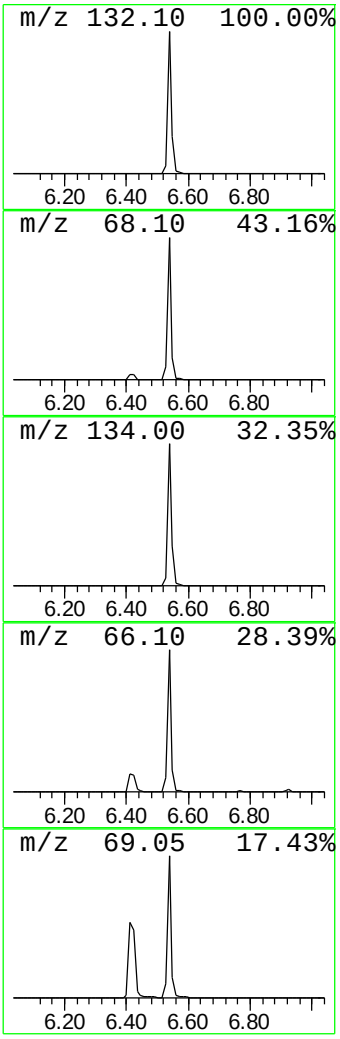
Peak Number 2 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	57.43 ng	1721100	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Data File : BF082431.D
Acq On : 22 Oct 2015 5:06
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

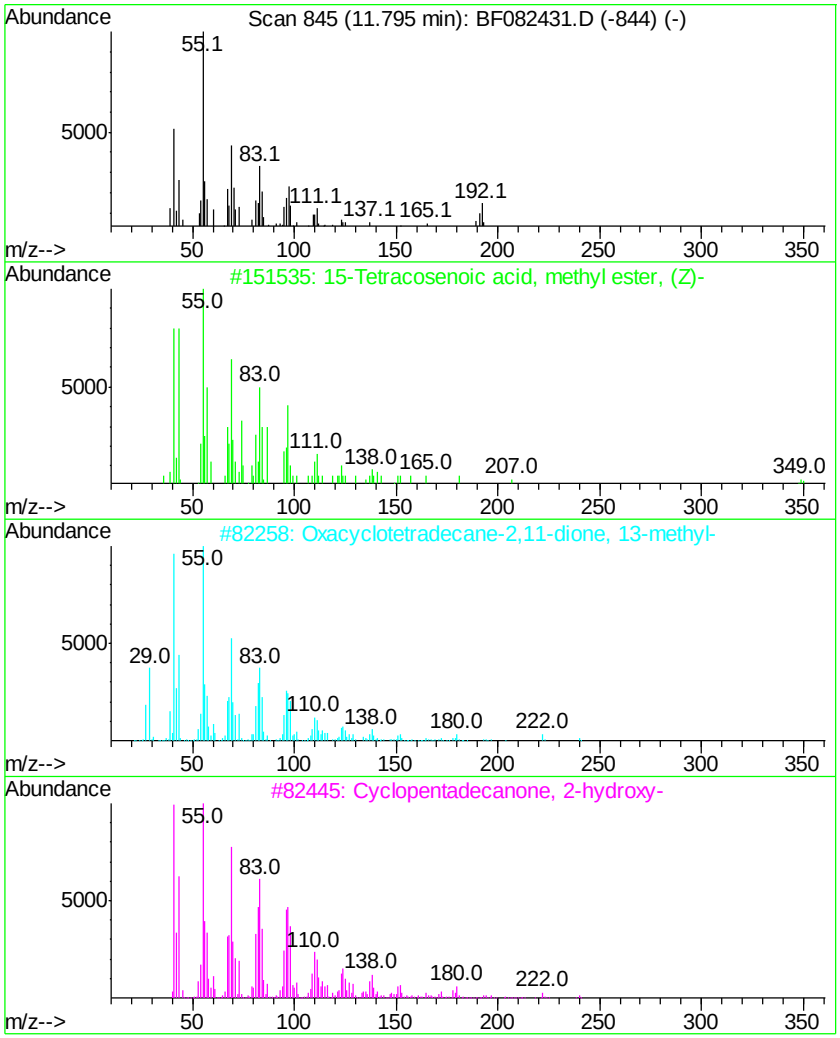
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

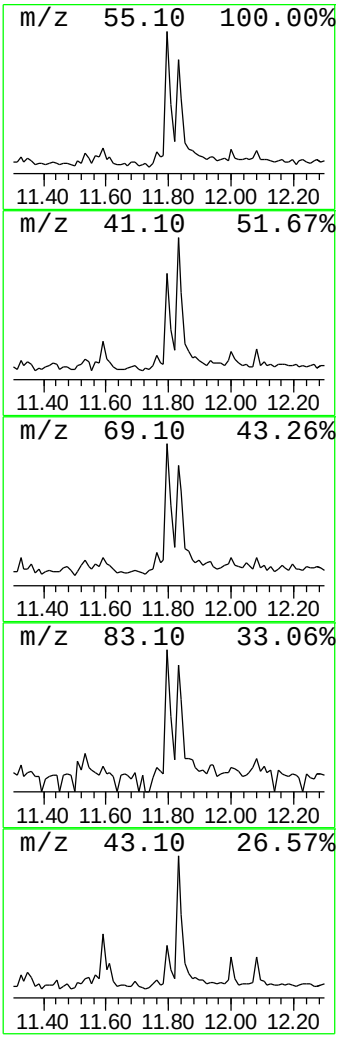
****

Peak Number 4 15-Tetracosenoic acid, meth... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.30 ng	74565	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Tetracosenoic acid, methyl es...	380	C25H48O2	002733-88-2	64
2	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	58
3	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	47
4	Chloromethyl 11-chlorododecanoate	282	C13H24Cl2O2	080419-07-4	47
5	1-Tridecene	182	C13H26	002437-56-1	46





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Sample : G4116-13
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ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

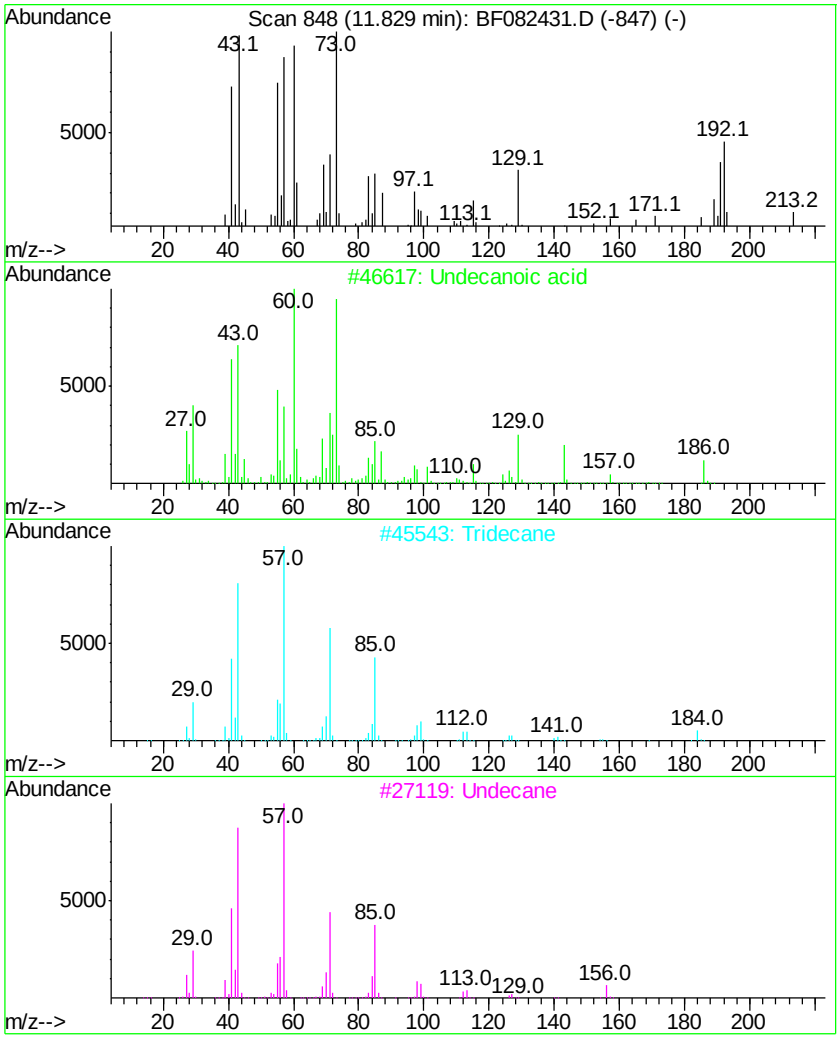
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

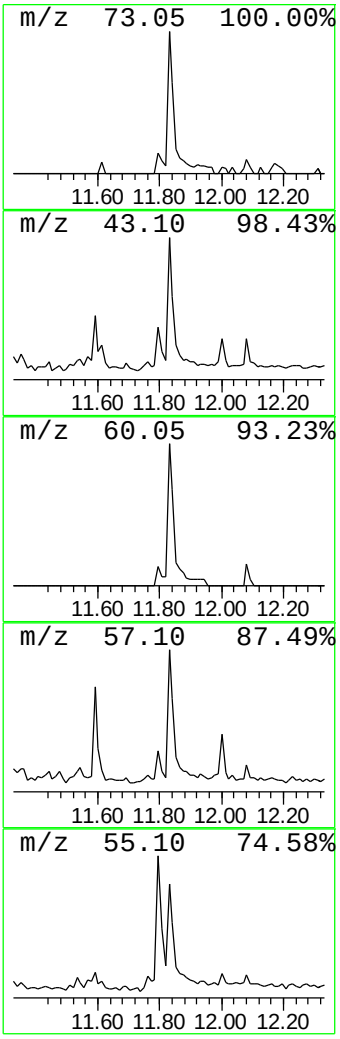
****

Peak Number 5 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	4.19 ng	135650	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	59
2	Tridecane	184	C13H28	000629-50-5	11
3	Undecane	156	C11H24	001120-21-4	11
4	Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	10
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	10





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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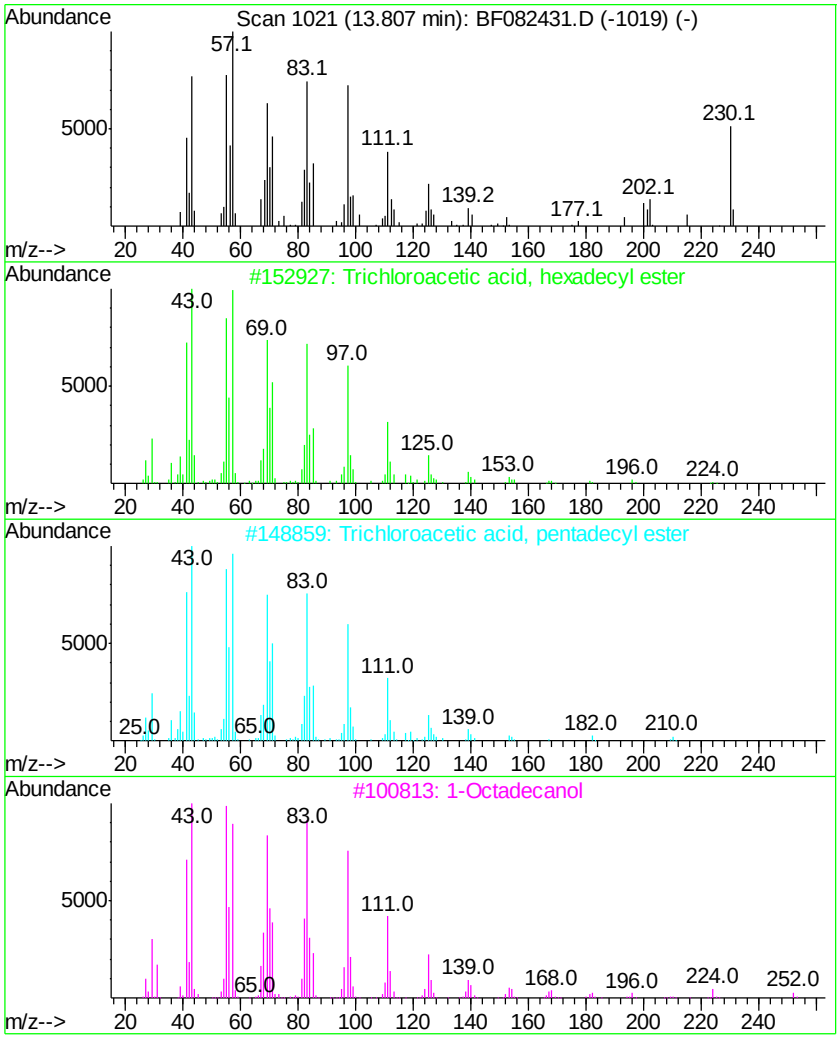
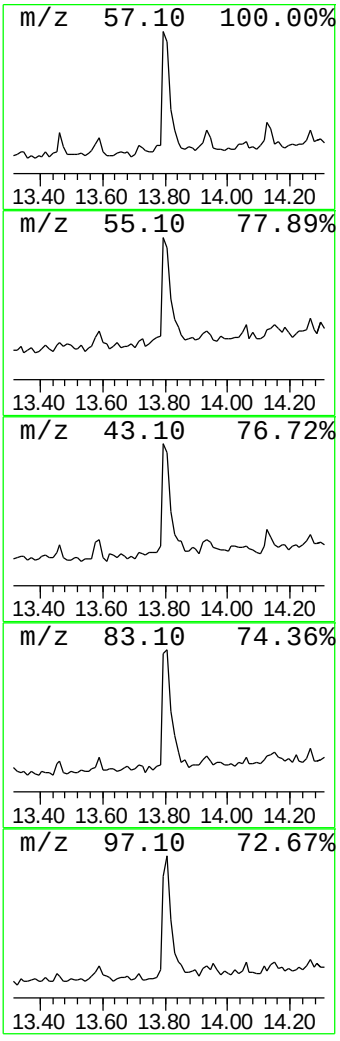
Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.29 ng	136154	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
3	1-Octadecanol	270	C18H38O	000112-92-5	76
4	1-Nonadecene	266	C19H38	018435-45-5	76
5	11-Tricosene	322	C23H46	052078-56-5	74





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Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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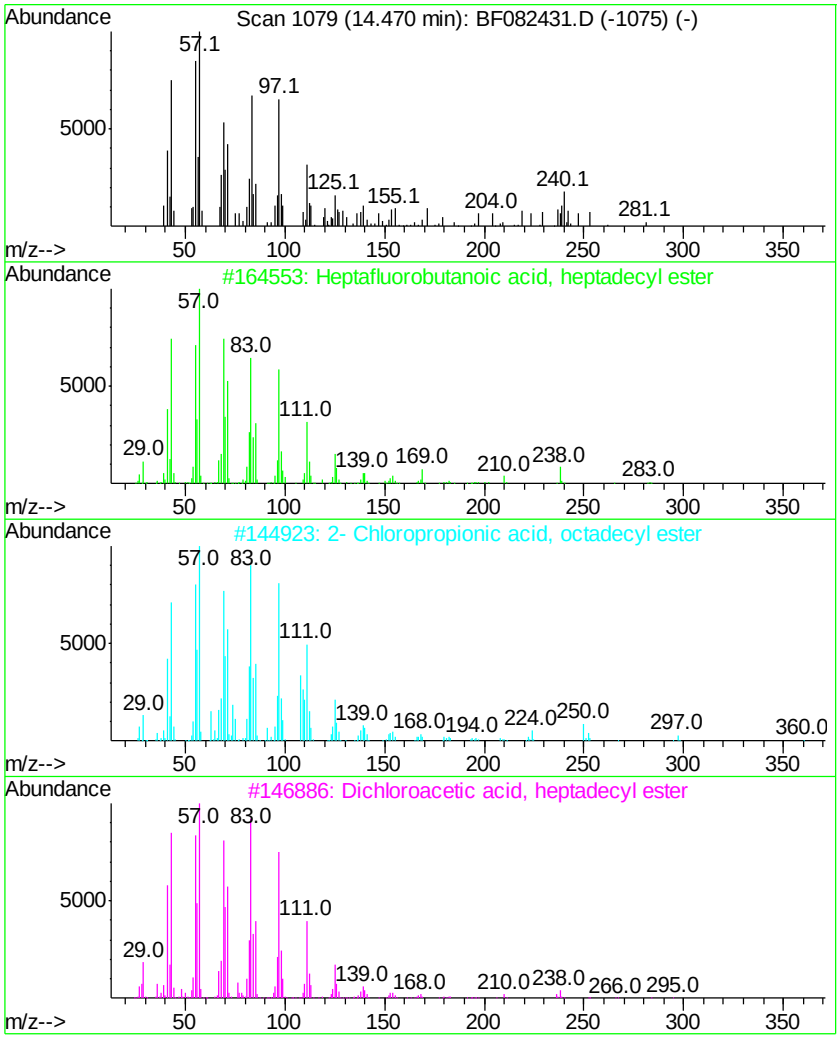
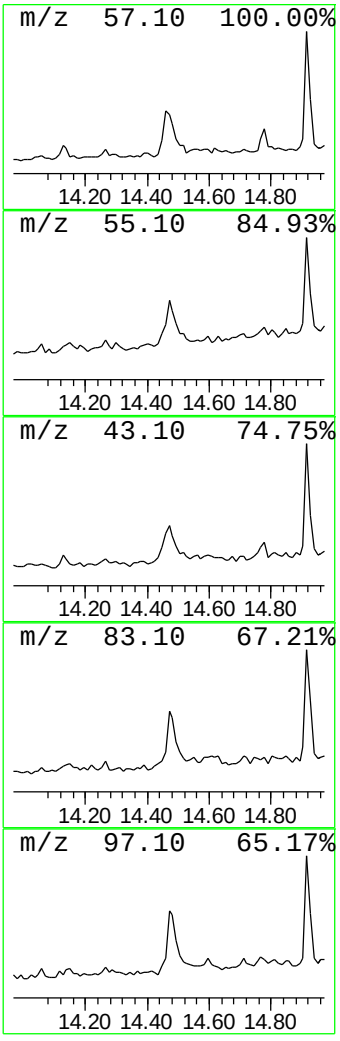
Peak Number 7 Heptafluorobutanoic acid, h... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	4.37 ng	180708	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	81
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	74
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	74
5	1-Docosene	308	C22H44	001599-67-3	72





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Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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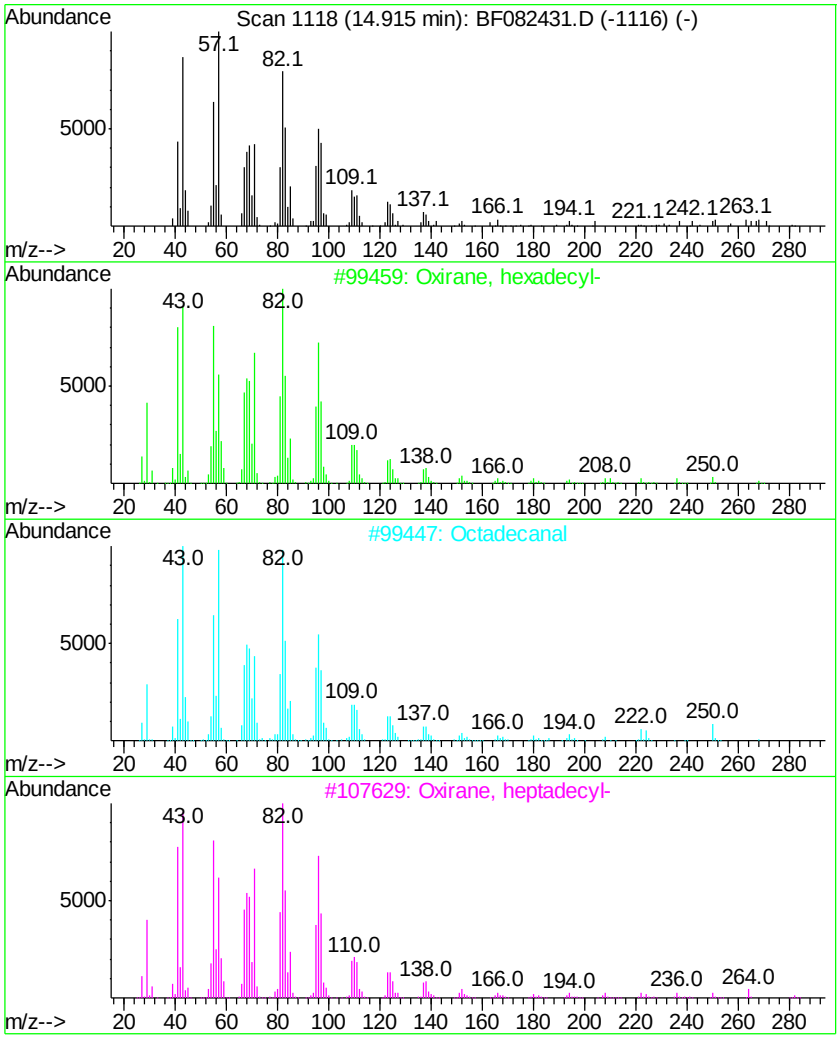
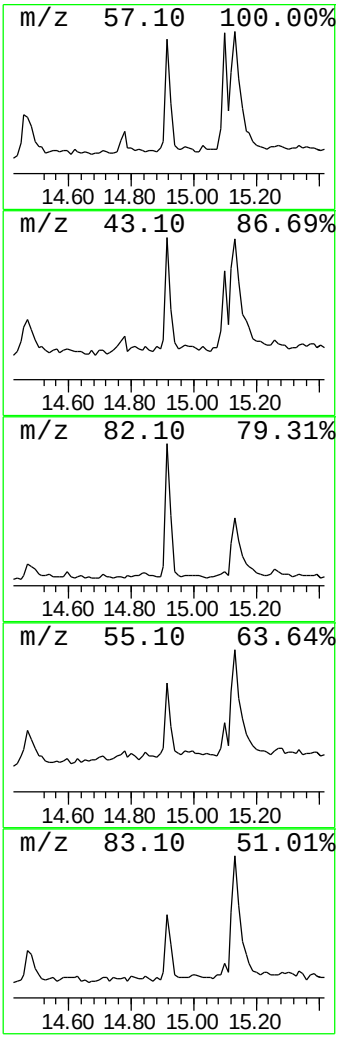
Peak Number 8 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	4.36 ng	156834	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	93
2	Octadecanal	268	C18H36O	000638-66-4	90
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
4	17-Octadecenal	266	C18H34O	056554-86-0	86
5	1,19-Eicosadiene	278	C20H38	014811-95-1	81





Library Search Compound Report

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Data File : BF082431.D
Acq On : 22 Oct 2015 5:06
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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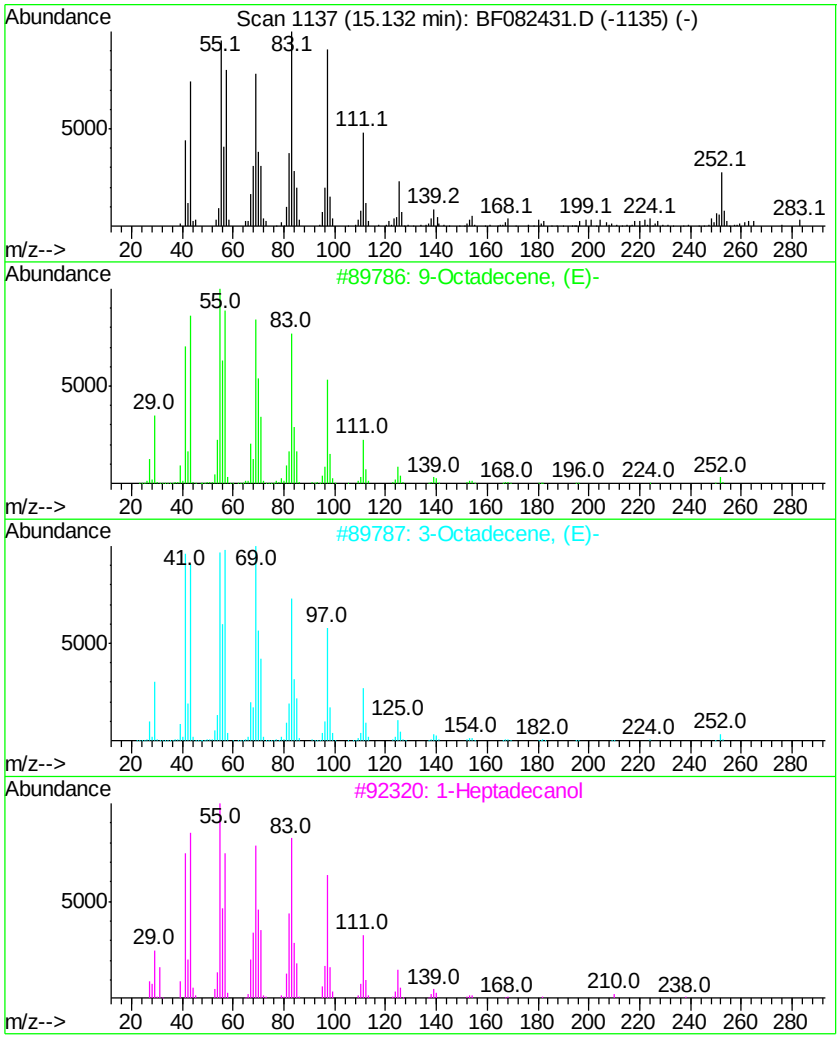
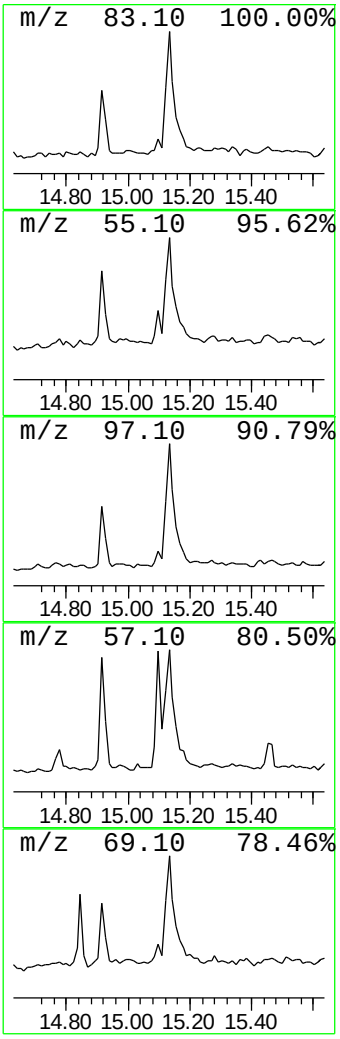
Peak Number 9 9-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.13	7.39 ng	266032	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecene, (E)-	252	C18H36	007206-25-9	94
2	3-Octadecene, (E)-	252	C18H36	007206-19-1	93
3	1-Heptadecanol	256	C17H36O	001454-85-9	76
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	70
5	1-Octadecanol	270	C18H38O	000112-92-5	70





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102115\
Data File : BF082431.D
Acq On : 22 Oct 2015 5:06
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

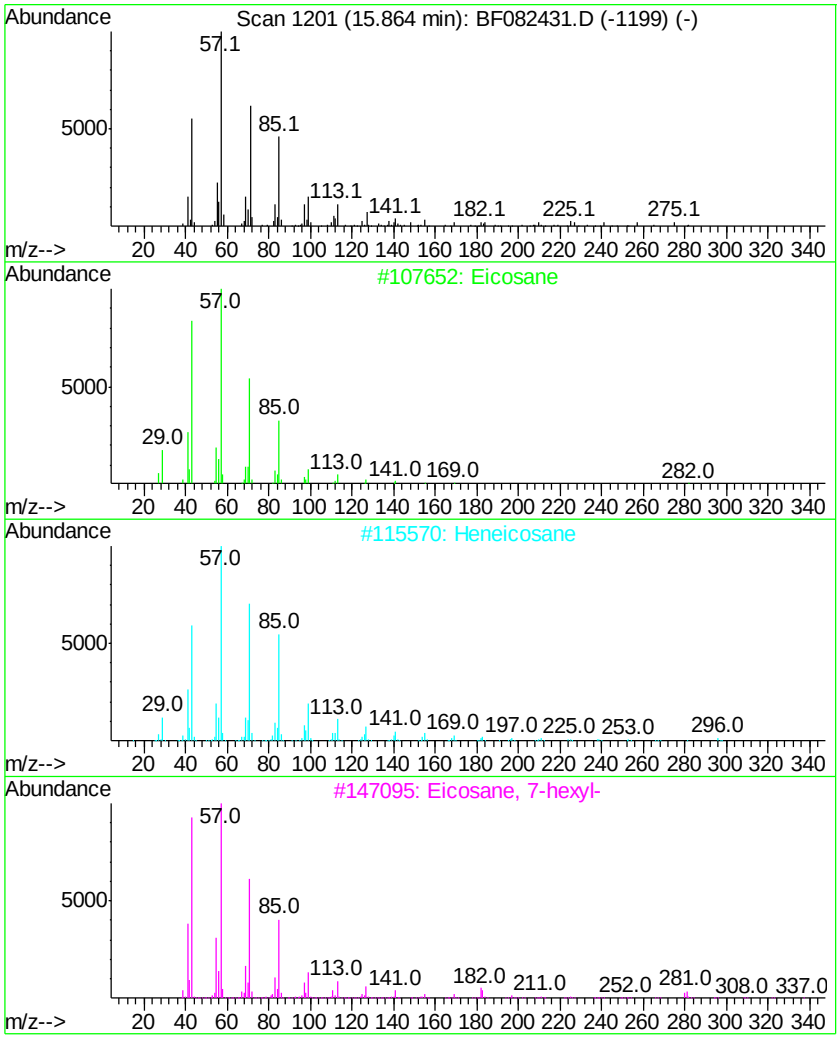
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

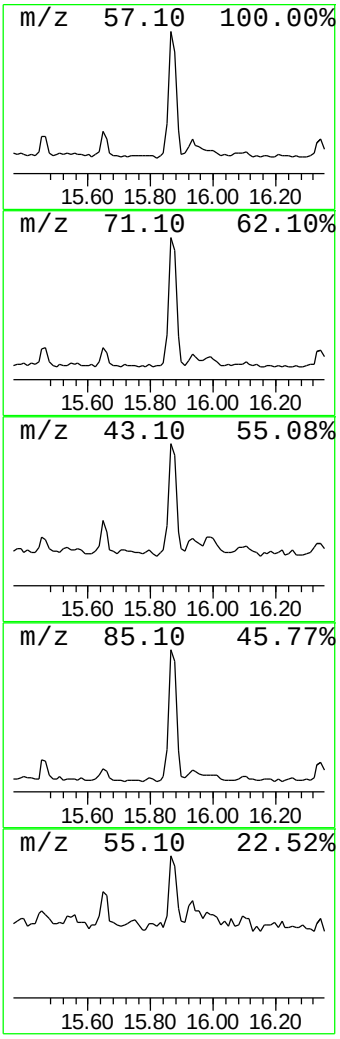
****

Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	4.14 ng	149132	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane	296	C21H44	000629-94-7	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102115\
Data File : BF082431.D
Acq On : 22 Oct 2015 5:06
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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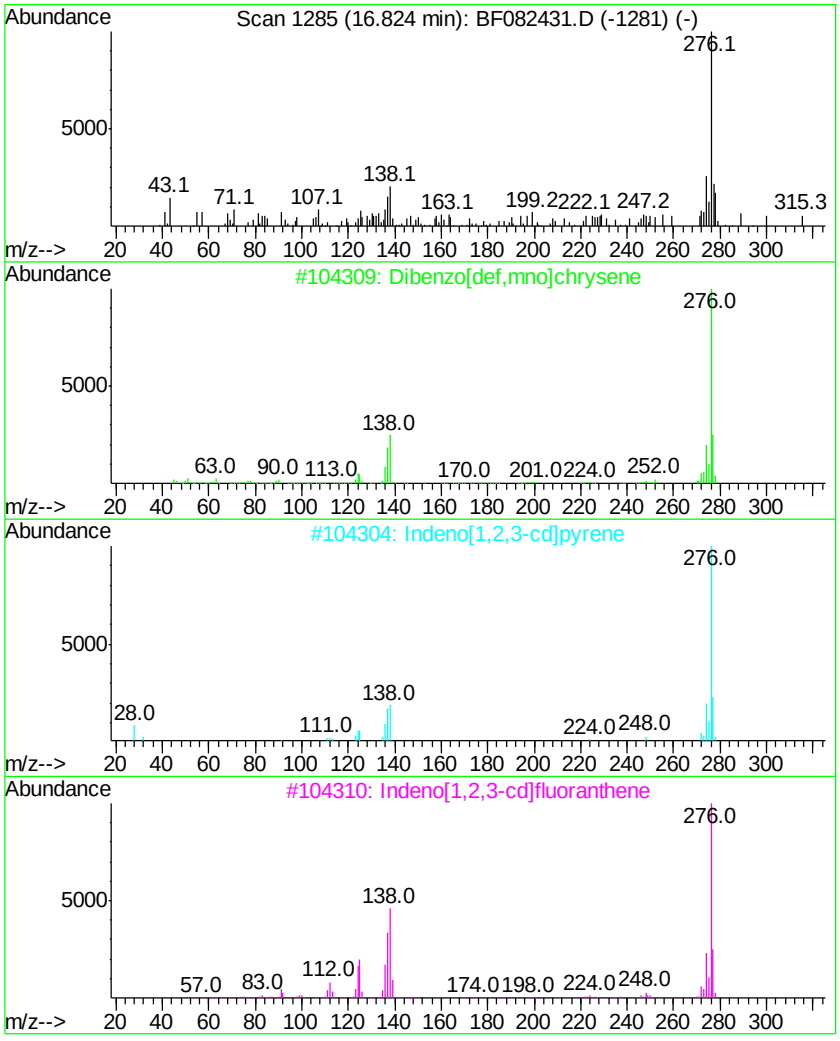
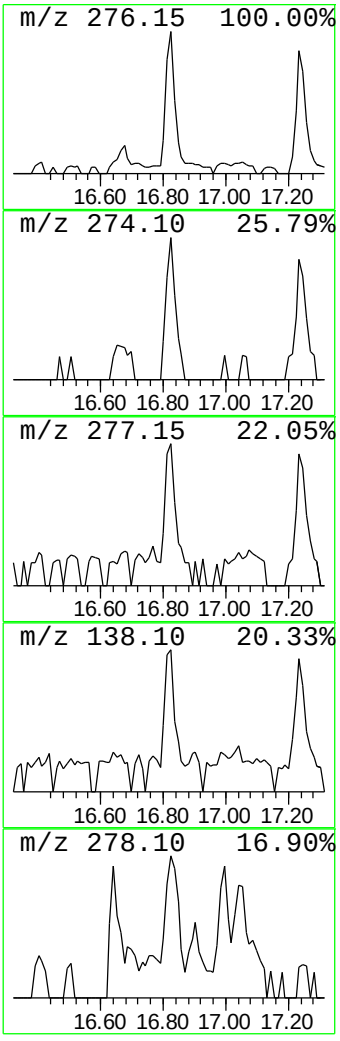
Peak Number 11 Dibenzo[def,mno]chrysene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.82	3.18 ng	114382	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	93
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	89
3	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	89
4	2-Thiophenecarbaldehyde, 5-[5-(t...	276	C13H8OS3	1000217-28-5	86
5	Benzo[ghi]perylene	276	C22H12	000191-24-2	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102115\
Data File : BF082431.D
Acq On : 22 Oct 2015 5:06
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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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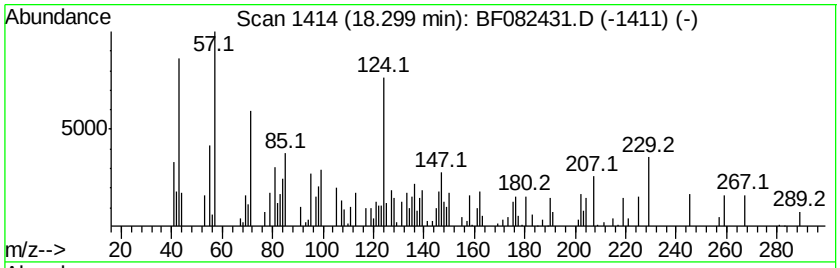
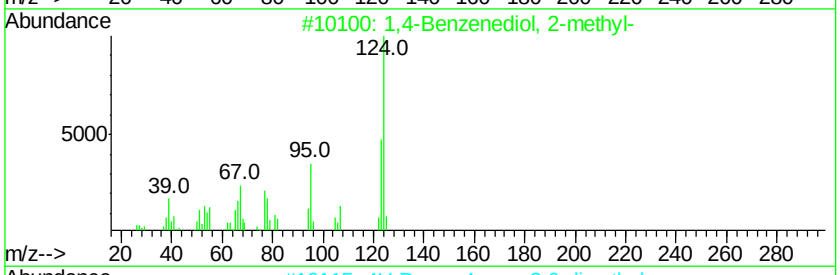
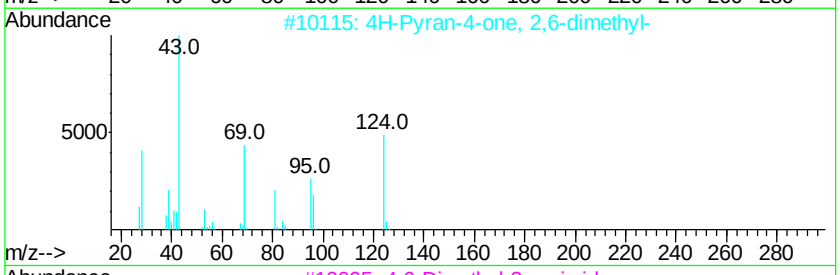
Peak Number 12 unknown18.30 Concentration Rank 9

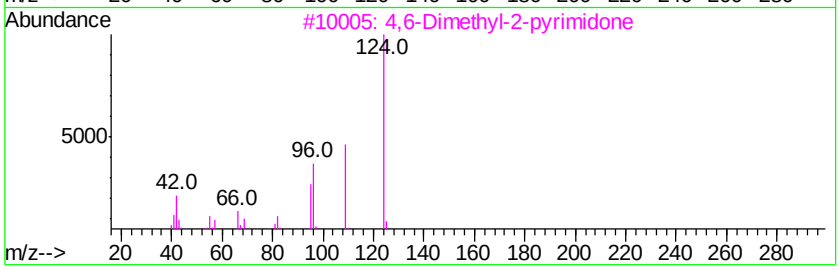
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.49 ng	125511	Perylene-d12	15.43

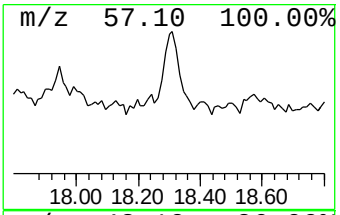
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenediol, 2-methyl-	124	C7H8O2	000095-71-6	27
2	4H-Pyran-4-one, 2,6-dimethyl-	124	C7H8O2	001004-36-0	27
3	4,6-Dimethyl-2-pyrimidone	124	C6H8N2O	000108-79-2	27
4	Phenol, 3-methoxy-	124	C7H8O2	000150-19-6	27
5	Propanoic acid, 3-amino-3-(4-flu...	183	C9H10FNO2	000325-89-3	22

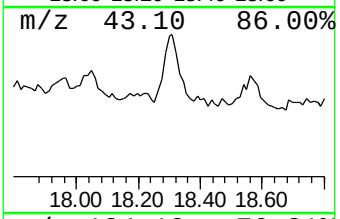


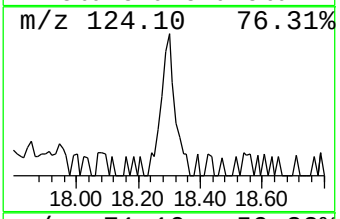


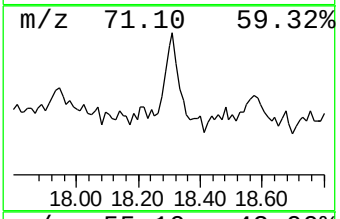


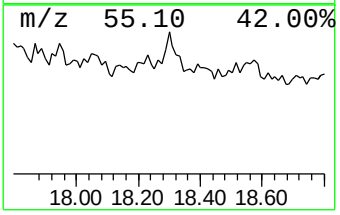












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102115\
Data File : BF082431.D
Acq On : 22 Oct 2015 5:06
Operator : UM/IZ
Sample : G4116-13
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BT-02(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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...	4.94	37.2	ng	1114370	1	6.77	599364	20.0
unknown6.54	6.54	57.4	ng	1721100	1	6.77	599364	20.0
15-Tetracosenoic ...	11.80	2.3	ng	74565	4	11.30	647374	20.0
Undecanoic acid	11.83	4.2	ng	135650	4	11.30	647374	20.0
Trichloroacetic a...	13.81	3.3	ng	136154	5	13.96	826677	20.0
Heptafluorobutano...	14.47	4.4	ng	180708	5	13.96	826677	20.0
Oxirane, hexadecyl-	14.92	4.4	ng	156834	6	15.43	720018	20.0
9-Octadecene, (E)-	15.13	7.4	ng	266032	6	15.43	720018	20.0
Eicosane	15.86	4.1	ng	149132	6	15.43	720018	20.0
Dibenzo[def,mno]c...	16.82	3.2	ng	114382	6	15.43	720018	20.0
unknown18.30	18.30	3.5	ng	125511	6	15.43	720018	20.0