LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082207.D
Acq On : 11 Oct 2015 6:40
Operator : UM/IZ
Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A10COMP

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	4.971	246	248	249	rBV	15704	17604	1.16%	0.106%
2	5.017	249	252	263	rVB	660261	849385	56.10%	5.119%
3	5.440	286	289	291	rBV	1221765	1409918	93.13%	8.498%
4	6.469	377	379	382	rBV	1004682	1297899	85.73%	7.823%
5	6.606	389	391	393	rBV	1630874	1513942	100.00%	9.125%
6	6.835	409	411	414	rBV	483141	464416	30.68%	2.799%
7	6.995	422	425	427	rBV	1344077	1212772	80.11%	7.310%
8	7.406	458	461	463	rBV	900134	849170	56.09%	5.118%
9	7.497	468	469	475	rVB	10895	20382	1.35%	0.123%
10	8.126	521	524	526	rBV	682370	612337	40.45%	3.691%
11	9.200	616	618	621	rBV	1653854	1512679	99.92%	9.117%
12	9.601	650	653	655	rBV	375164	319880	21.13%	1.928%
13	9.875	675	677	680	rBV	477035	674800	44.57%	4.067%
14	10.309	711	715	716	rBV	34634	47912	3.16%	0.289%
15	10.526	731	734	737	rBV2	11531	16608	1.10%	0.100%
16	10.675	744	747	749	rBV2	688957	888338	58.68%	5.354%
17	10.778	754	756	763	rVB	44607	56143	3.71%	0.338%
18	11.224	793	795	797	rBV	30312	34470	2.28%	0.208%
19	11.361	805	807	810	rBV	446801	585537	38.68%	3.529%
20	11.658	831	833	834	rBV	19557	20410	1.35%	0.123%
21	11.864	849	851	852	rBV	48066	43180	2.85%	0.260%
22	11.898	852	854	856	rBV	46387	55473	3.66%	0.334%
23	12.092	870	871	874	rVB2	48044	57598	3.80%	0.347%
24	12.389	895	897	901	rBV4	39980	39864	2.63%	0.240%
25	12.572	911	913	917	rVB	47968	87920	5.81%	0.530%
26	12.641	917	919	920	rBV	70297	61801	4.08%	0.372%
27	12.664	920	921	924	rVB2	222009	232096	15.33%	1.399%
28	12.767	928	930	936	rBV3	293832	512368	33.84%	3.088%
29	12.892	939	941	942	rVB	45728	40779	2.69%	0.246%
30	12.949	944	946	949	rBV	1167021	1125390	74.34%	6.783%
31	13.224	967	970	972	rVB2	12045	16240	1.07%	0.098%
32	13.269	972	974	978	rVB3	34208	37684	2.49%	0.227%
33	13.407	984	986	987	rBV	14652	19114	1.26%	0.115%
34	13.429	987	988	990	rVV	71819	63919	4.22%	0.385%

LSC Area Percent Report

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Data File : BF082207.D
Acq On : 11 Oct 2015 6:40
Operator : UM/IZ
Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A10COMP

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	13.475	990	992	994	rVB	36920	31979	2.11%	0.193%
36	13.852	1023	1025	1031	rBV	91232	146878	9.70%	0.885%
37	14.001	1036	1038	1045	rVB	426524	554427	36.62%	3.342%
38	14.161	1050	1052	1056	rVB	10560	16805	1.11%	0.101%
39	14.470	1077	1079	1086	rBV3	23144	66477	4.39%	0.401%
40	14.767	1102	1105	1107	rBV2	15564	24542	1.62%	0.148%
41	14.835	1109	1111	1114	rVB2	14740	18589	1.23%	0.112%
42	15.030	1125	1128	1131	rBV	29179	60294	3.98%	0.363%
43	15.087	1131	1133	1135	rVV	28784	41984	2.77%	0.253%
44	15.133	1135	1137	1139	rVB2	14258	18838	1.24%	0.114%
45	15.315	1151	1153	1156	rBV	20987	29005	1.92%	0.175%
46	15.384	1156	1159	1161	rVV	19107	30157	1.99%	0.182%
47	15.441	1161	1164	1170	rVV	383204	499095	32.97%	3.008%
48	15.647	1180	1182	1189	rVB4	10380	21619	1.43%	0.130%
49	15.875	1199	1202	1205	rBV	43421	67900	4.48%	0.409%
50	15.933	1205	1207	1210	rBV3	13795	29891	1.97%	0.180%
51	16.847	1284	1287	1290	rBV2	13689	32806	2.17%	0.198%
52	16.916	1290	1293	1297	rVB3	10207	23535	1.55%	0.142%
53	17.270	1320	1324	1327	rBV2	7227	18221	1.20%	0.110%
54	17.396	1330	1335	1338	rBV6	7420	25729	1.70%	0.155%
55	18.356	1416	1419	1424	rVB4	7094	16413	1.08%	0.099%
56	19.361	1503	1507	1512	rVB6	7113	18478	1.22%	0.111%

Sum of corrected areas: 16591690

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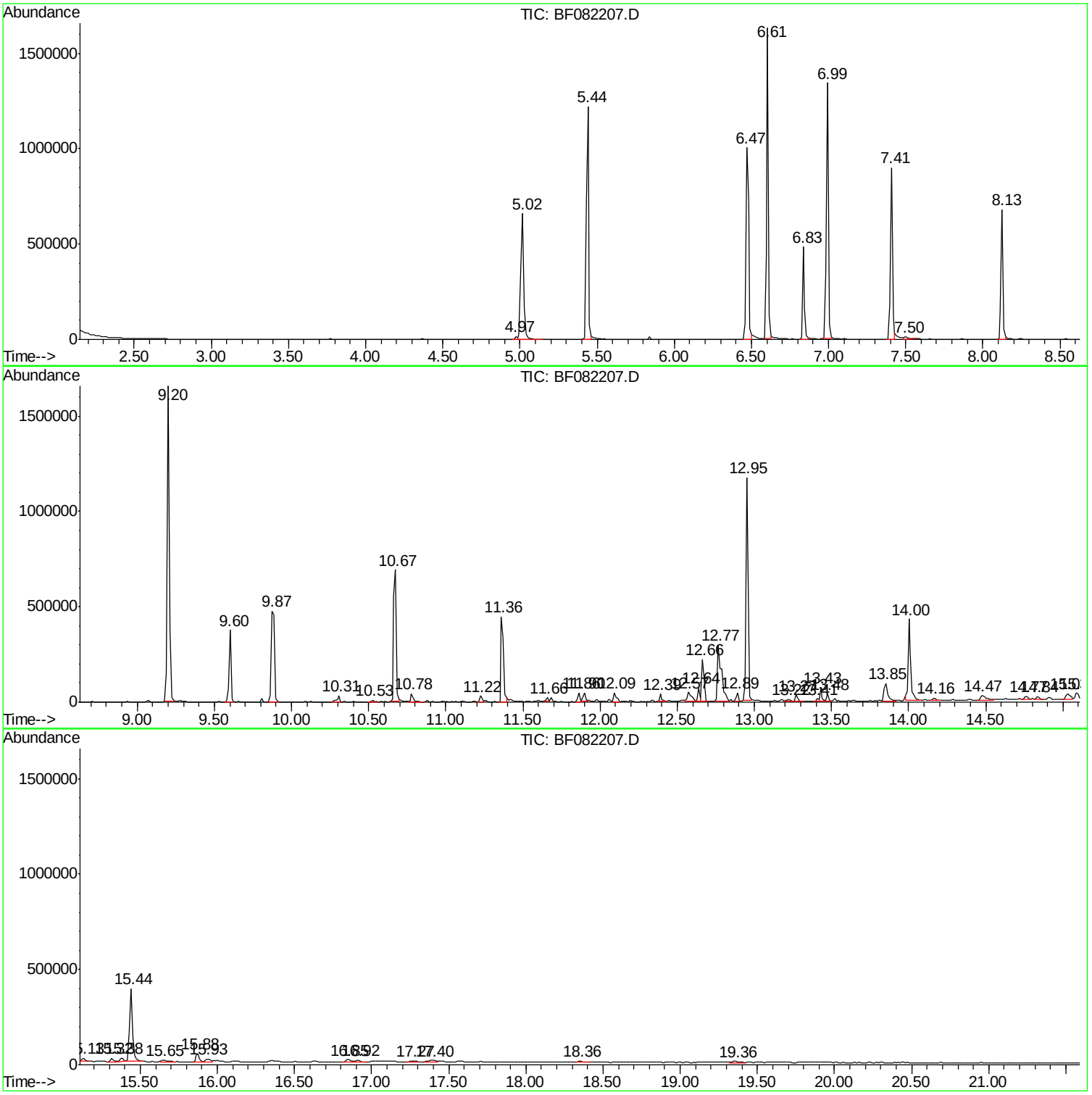
Data File : BF082207.D
Acq On : 11 Oct 2015 6:40
Operator : UM/IZ
Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A10COMP

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082207.D
Acq On : 11 Oct 2015 6:40
Operator : UM/IZ
Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

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

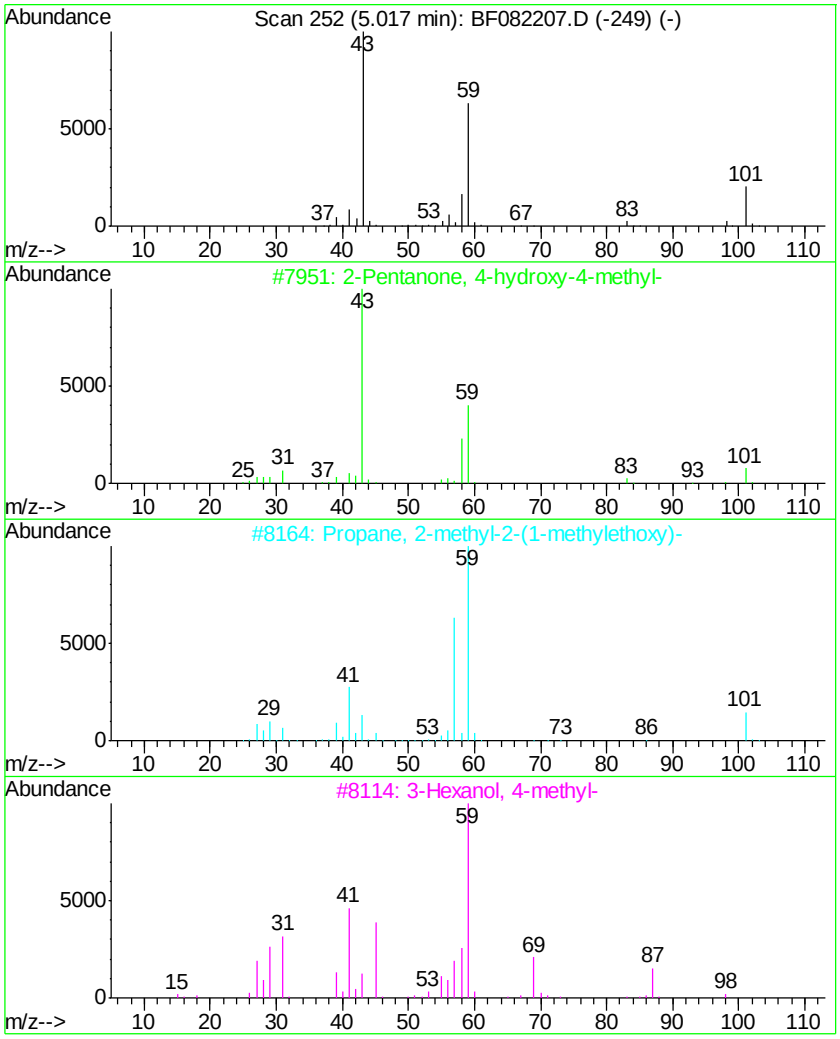
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

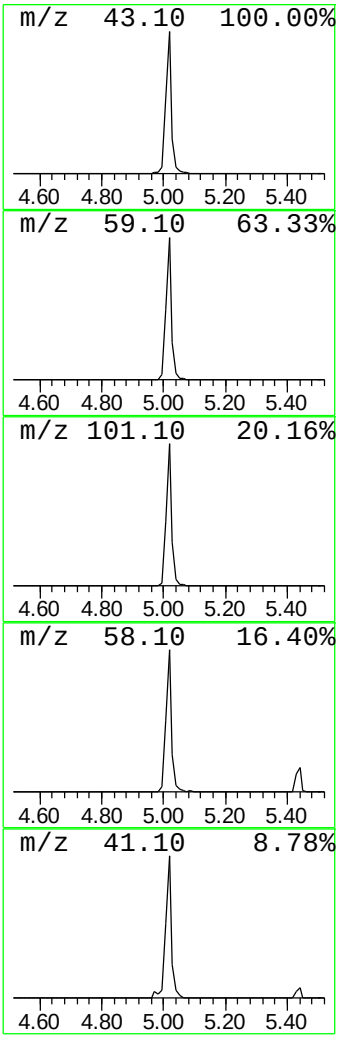
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	36.58 ng	849385	1,4-Dichlorobenzene-d4	6.83

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	28
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF082207.D
Acq On : 11 Oct 2015 6:40
Operator : UM/IZ
Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A10COMP

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

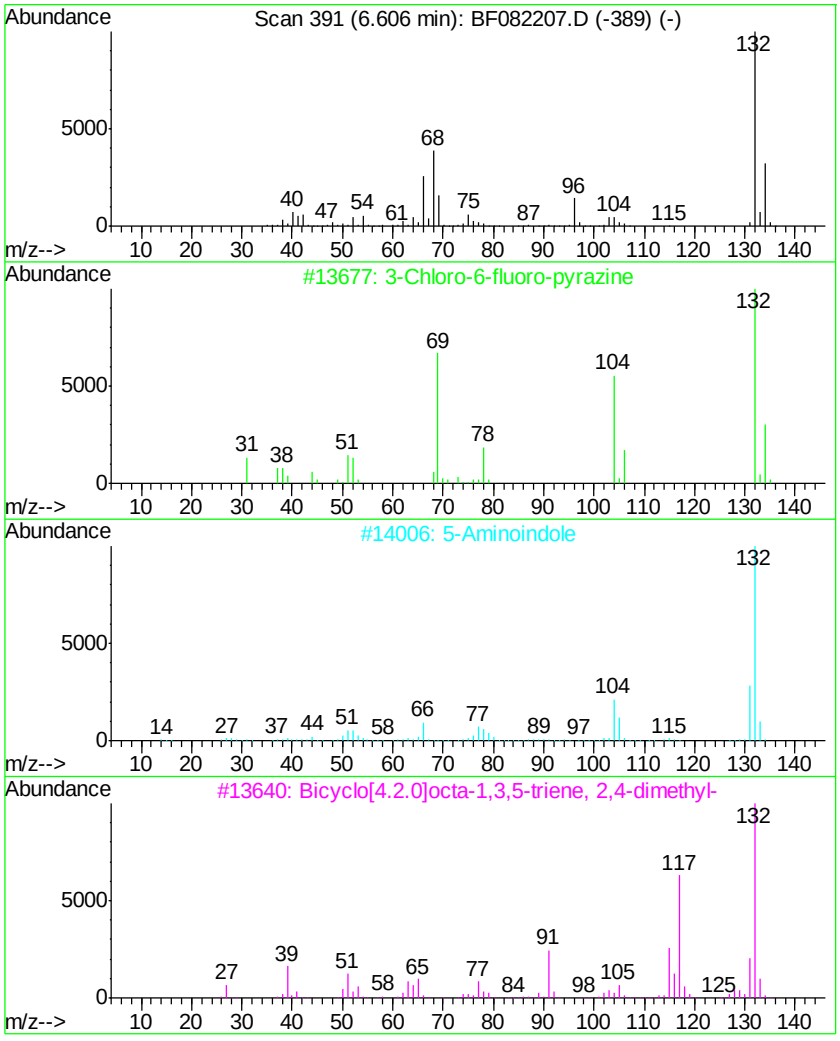
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

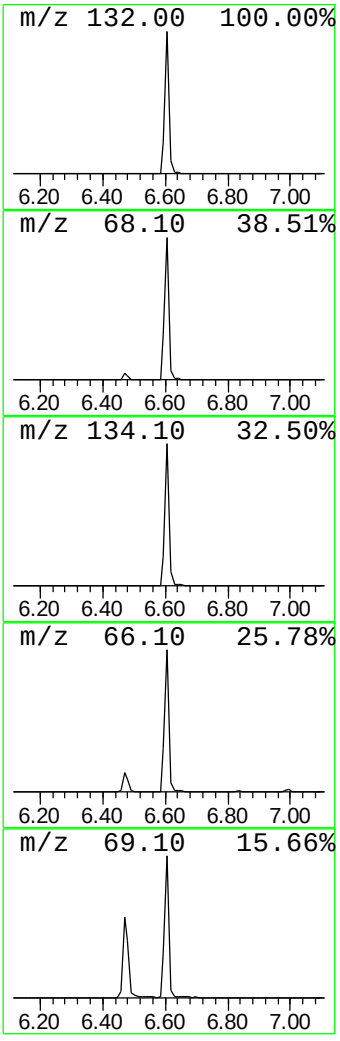
****

Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	65.20 ng	1513940	1,4-Dichlorobenzene-d4	6.83

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Data File : BF082207.D
Acq On : 11 Oct 2015 6:40
Operator : UM/IZ
Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A10COMP

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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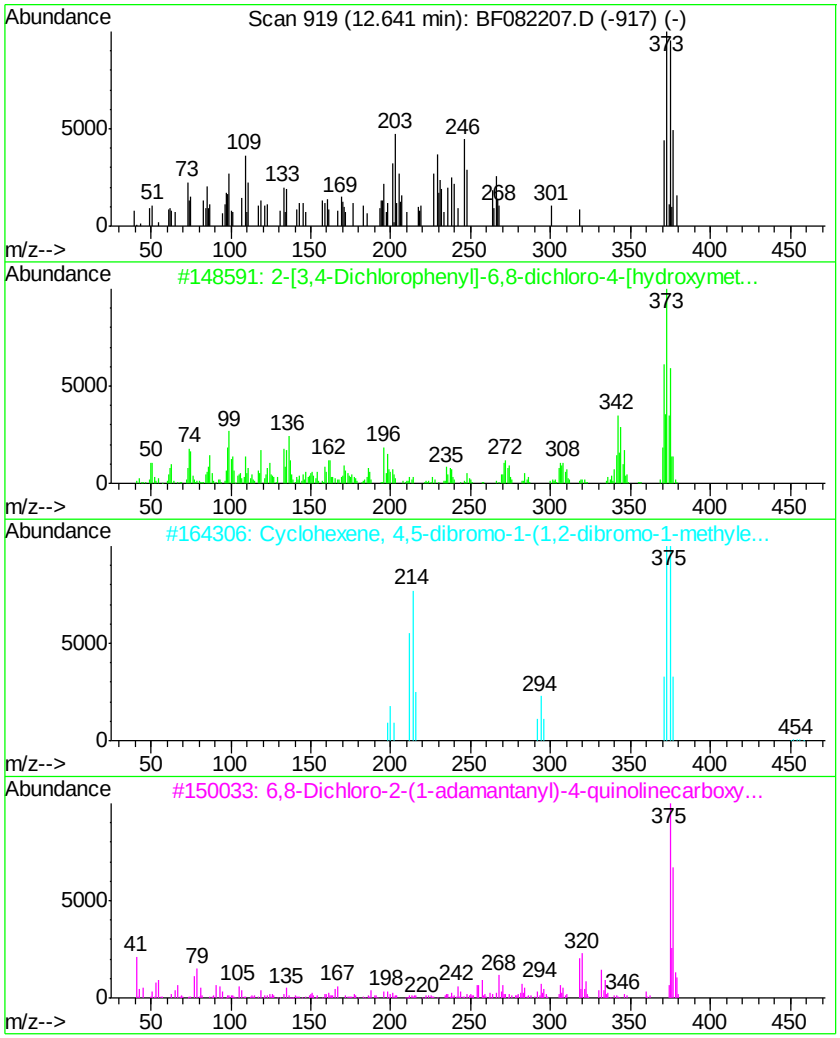
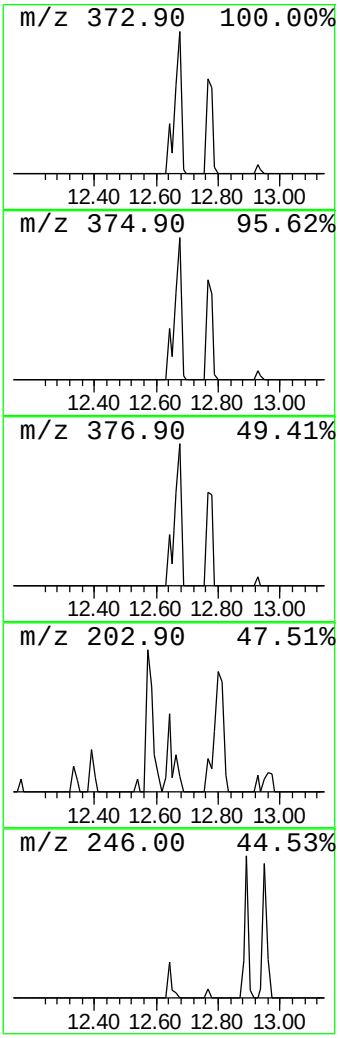
Peak Number 4 unknown12.64 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.11 ng	61801	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[3,4-Dichlorophenyl]-6,8-dichl...	371	C16H9Cl4NO	038599-01-8	43
2	Cyclohexene, 4,5-dibromo-1-(1,2-...	450	C10H14Br4	070168-60-4	28
3	6,8-Dichloro-2-(1-adamantanyl)-4...	375	C20H19Cl2NO2	049647-91-8	12
4	7-Fluoro-3,4-dihydro-3-[4-[trifl...	375	C20H13F4NO2	144155-10-2	10
5	2-Pyridyl-2-[p-chloroanilino]-6-...	373	C22H16ClN3O	050503-95-2	10





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Data File : BF082207.D
Acq On : 11 Oct 2015 6:40
Operator : UM/IZ
Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A10COMP

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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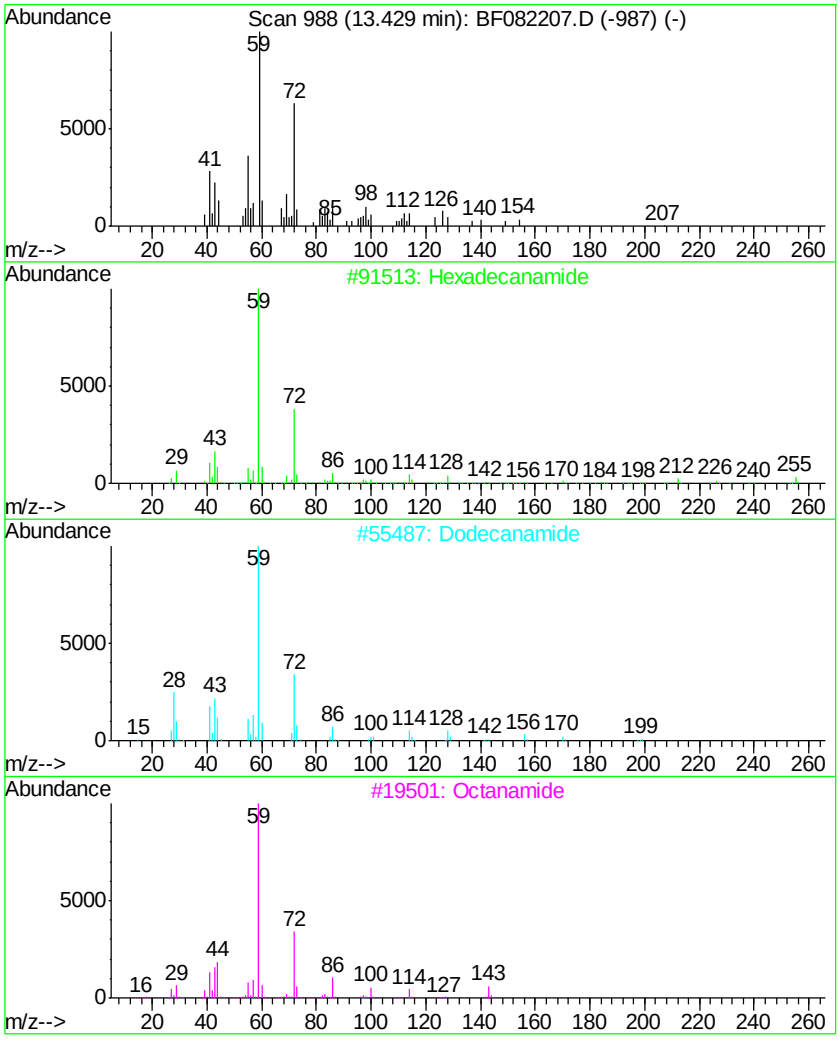
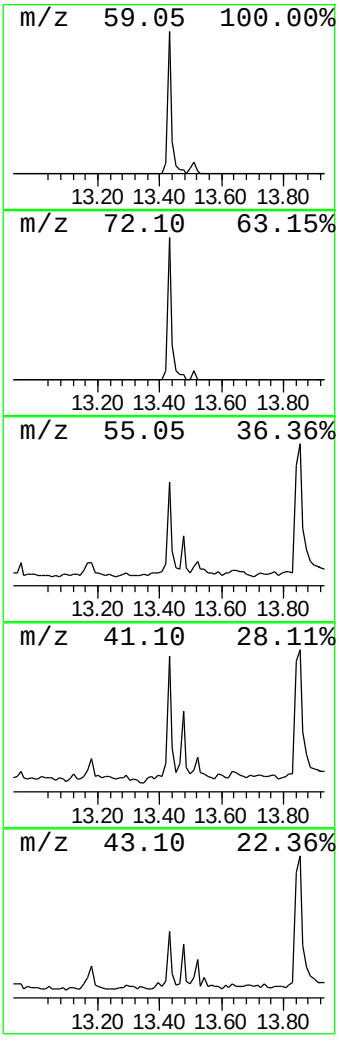
Peak Number 6 Hexadecanamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	2.31 ng	63919	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	72
2	Dodecanamide	199	C12H25NO	001120-16-7	59
3	Octanamide	143	C8H17NO	000629-01-6	50
4	Silane, hexyl-	116	C6H16Si	001072-14-6	47
5	Tetradecanamide	227	C14H29NO	000638-58-4	45





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TIC Library : C:\DATABASE\NIST02.L
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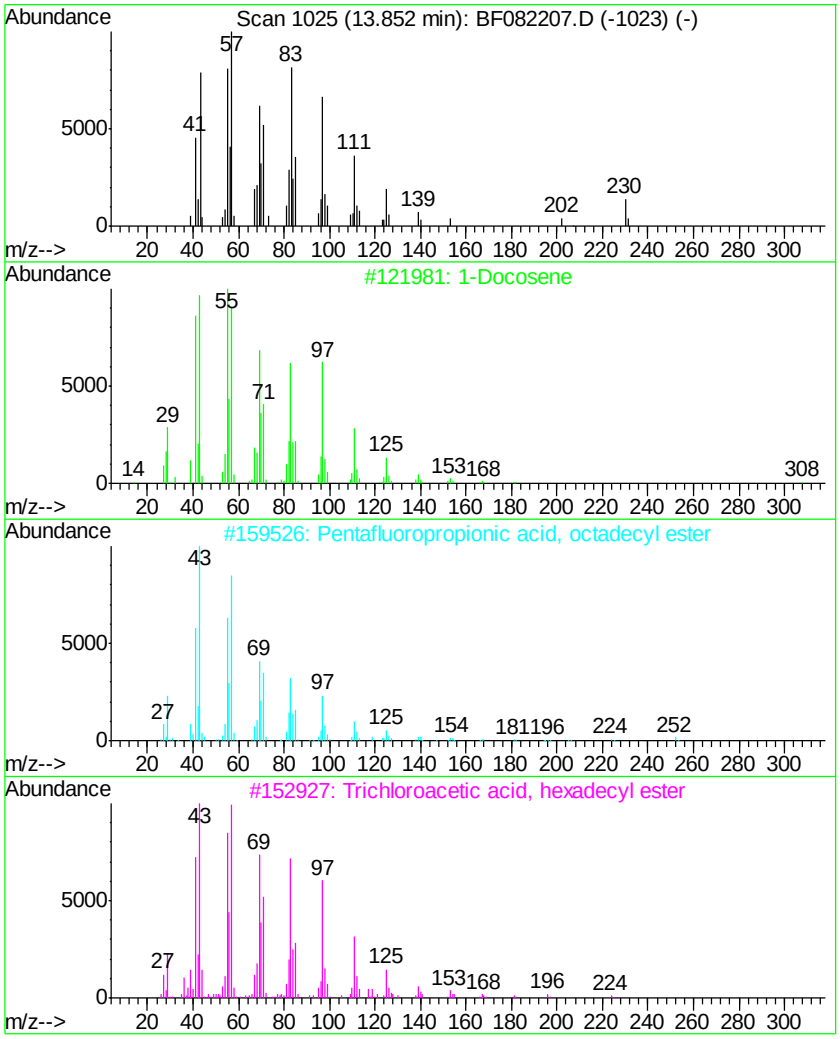
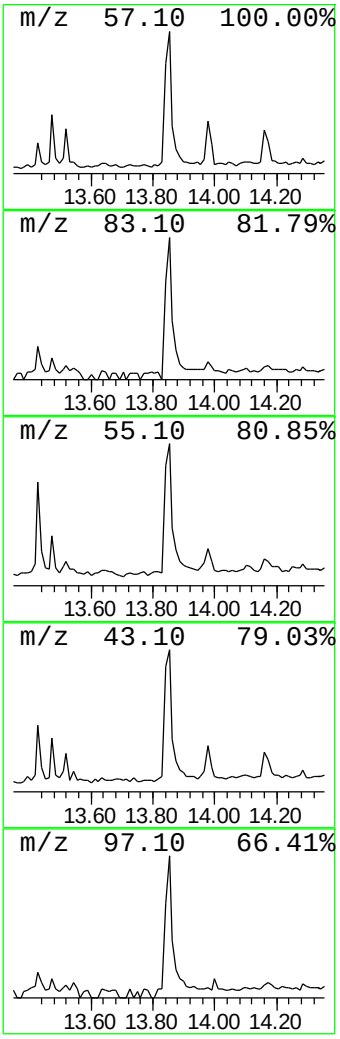
Peak Number 7 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	5.30 ng	146878	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	90
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	90
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4	17-Pentatriacontene	491	C35H70	006971-40-0	87
5	1-Octadecanol	270	C18H38O	000112-92-5	87





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Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A10COMP

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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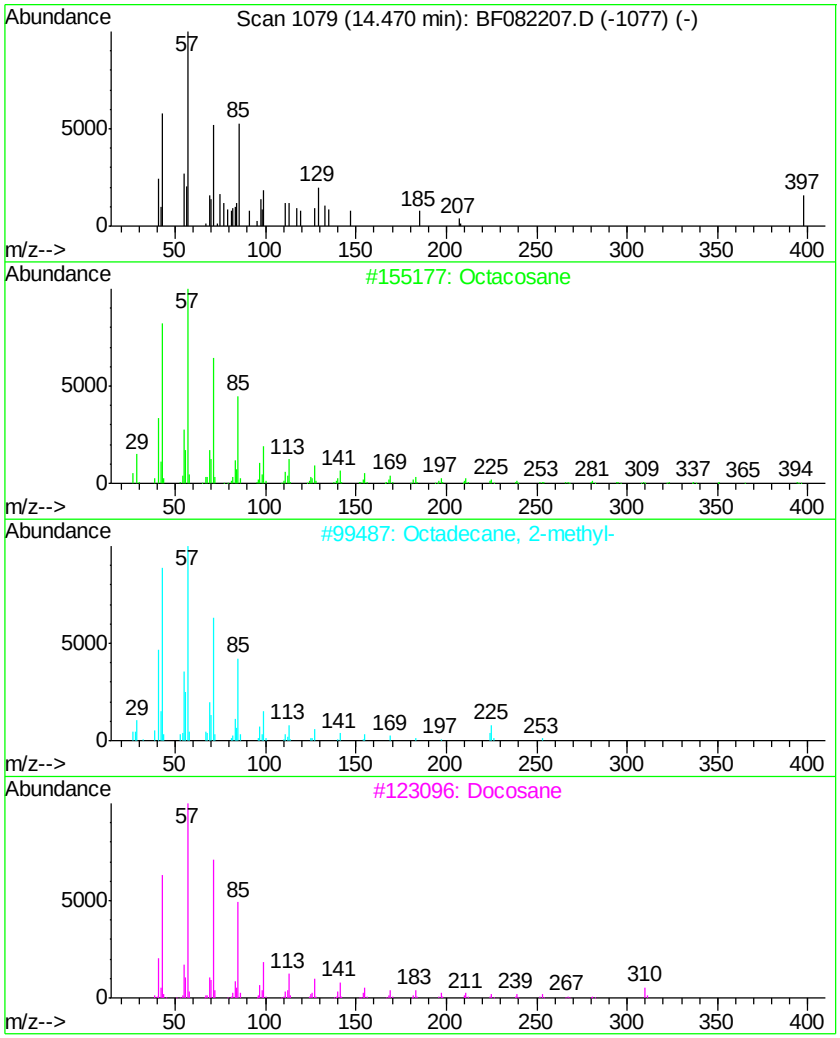
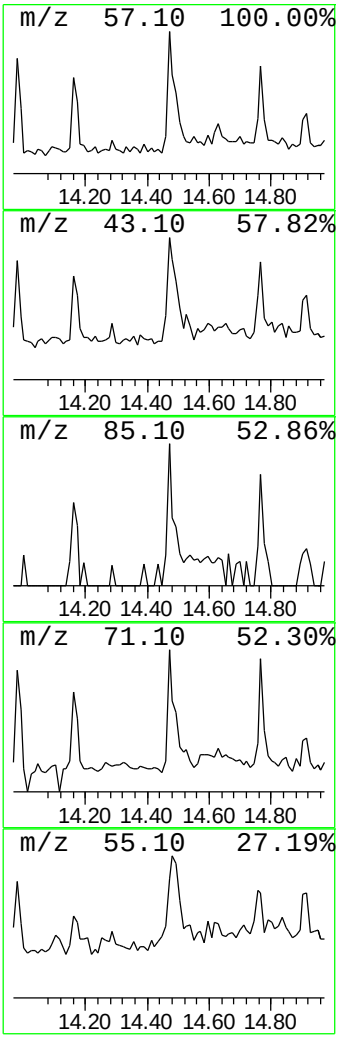
Peak Number 8 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.40 ng	66477	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	52
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	50
3	Docosane	310	C22H46	000629-97-0	50
4	Eicosane	282	C20H42	000112-95-8	50
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	50





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Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A10COMP

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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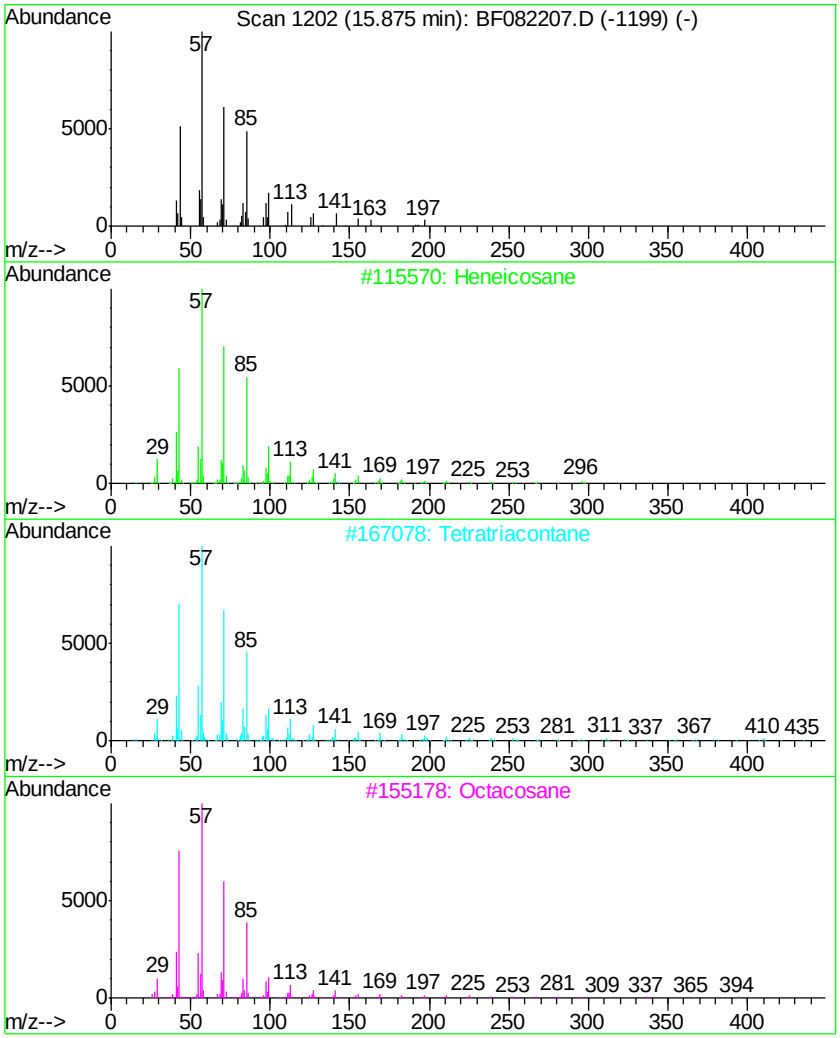
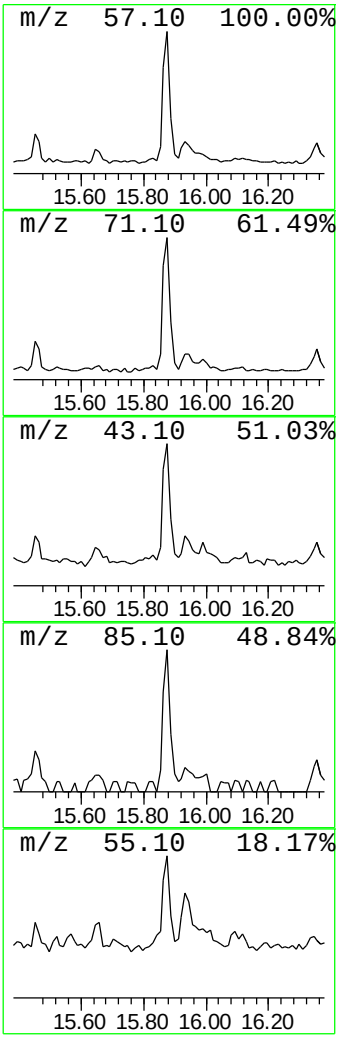
Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	2.72 ng	67900	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetratriacontane	479	C34H70	014167-59-0	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082207.D
Acq On : 11 Oct 2015 6:40
Operator : UM/IZ
Sample : G3979-19
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A10COMP

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...	5.02	36.6	ng	849385	1	6.83	464416	20.0
unknown6.61	6.61	65.2	ng	1513940	1	6.83	464416	20.0
unknown12.64	12.64	2.1	ng	61801	4	11.36	585537	20.0
Hexadecanamide	13.43	2.3	ng	63919	5	14.00	554427	20.0
1-Docosene	13.85	5.3	ng	146878	5	14.00	554427	20.0
Octacosane	14.47	2.4	ng	66477	5	14.00	554427	20.0
Heneicosane	15.88	2.7	ng	67900	6	15.44	499095	20.0