LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

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-BF100516.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	5.194	247	250	260	rVB	1315031	1901185	25.69%	2.836%
2	5.606	283	286	288	rBV	5654779	6730028	90.96%	10.039%
3	6.577	368	371	372	rBV	60865	110561	1.49%	0.165%
4	6.623	372	375	378	rVB	5406083	6872254	92.88%	10.251%
5	6.760	384	387	389	rBV	6885771	7069820	95.55%	10.545%
6	6.989	404	407	409	rBV	1717005	1608416	21.74%	2.399%
7	7.149	418	421	423	rVB	5585837	5954745	80.48%	8.882%
8	7.549	453	456	458	rBV	3827475	4324946	58.45%	6.451%
9	7.652	461	465	467	rVV	193072	324886	4.39%	0.485%
10	8.269	517	519	521	rBV	1705252	2129189	28.78%	3.176%
11	9.355	611	614	617	rBV	7791716	7399242	100.00%	11.037%
12	9.743	646	648	650	rBV	1804024	2219906	30.00%	3.311%
13	9.960	664	667	670	rVB	57802	77062	1.04%	0.115%
14	10.040	671	674	676	rVB	2089444	2454345	33.17%	3.661%
15	10.463	708	711	713	rBV	196599	216764	2.93%	0.323%
16	10.692	728	731	734	rBV	77880	144020	1.95%	0.215%
17	10.829	740	743	745	rBV	4844527	4727304	63.89%	7.051%
18	10.943	750	753	758	rVB	221225	342969	4.64%	0.512%
19	11.389	790	792	794	rBV	175797	173780	2.35%	0.259%
20	11.526	801	804	806	rBV	2707069	2337001	31.58%	3.486%
21	12.052	847	850	852	rBV	489806	501146	6.77%	0.748%
22	12.841	917	919	925	rBV	260424	360859	4.88%	0.538%
23	13.115	941	943	946	rBV	5400081	5893308	79.65%	8.790%
24	14.018	1019	1022	1027	rBV	190096	313497	4.24%	0.468%
25	14.167	1033	1035	1038	rBV	1095779	1380709	18.66%	2.059%
26	15.675	1164	1167	1169	rBV	814173	1185716	16.02%	1.769%
27	16.407	1229	1231	1236	rVB2	77647	172130	2.33%	0.257%
28	16.864	1268	1271	1276	rVB	47209	116261	1.57%	0.173%

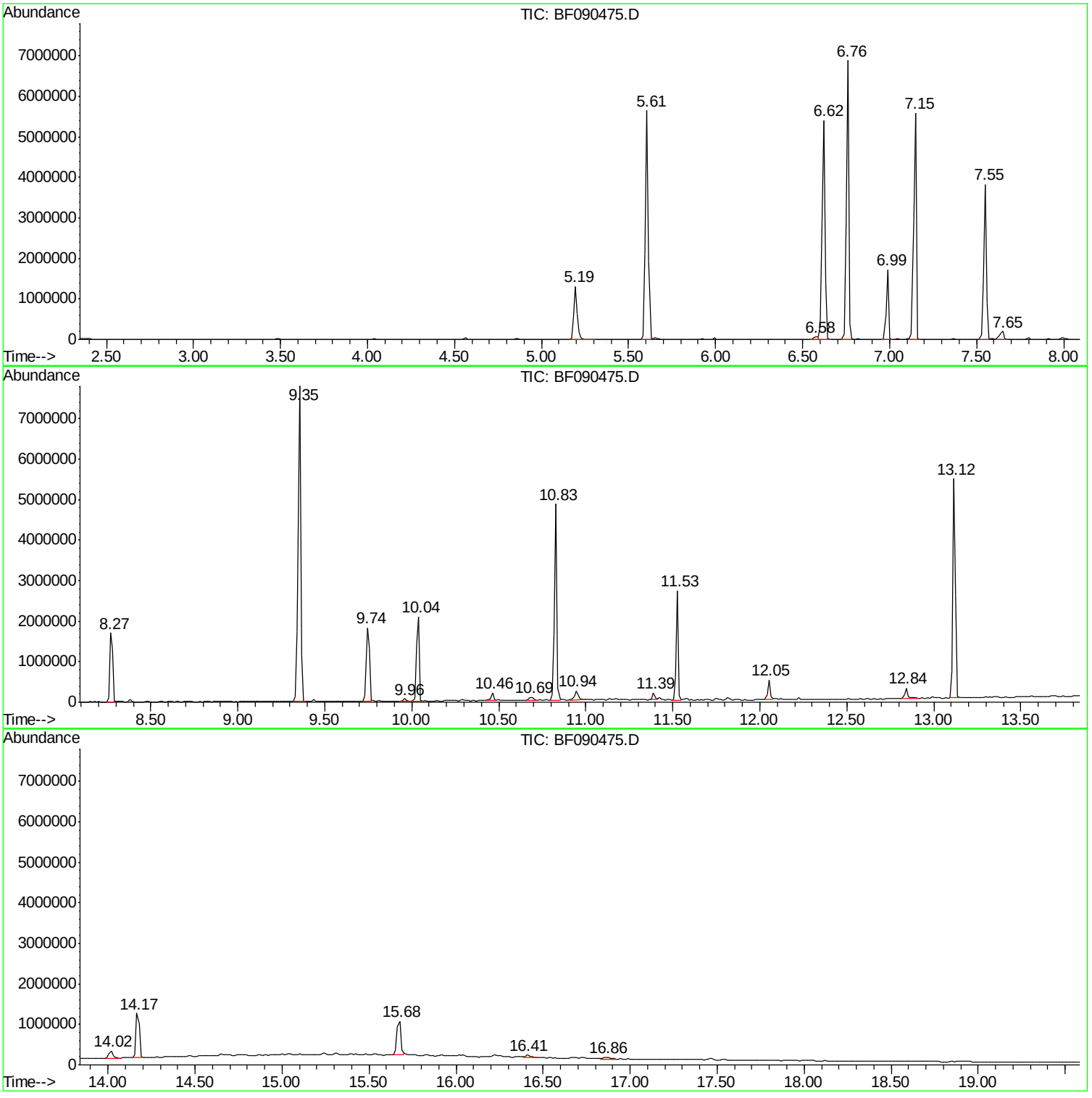
Sum of corrected areas: 67042049

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

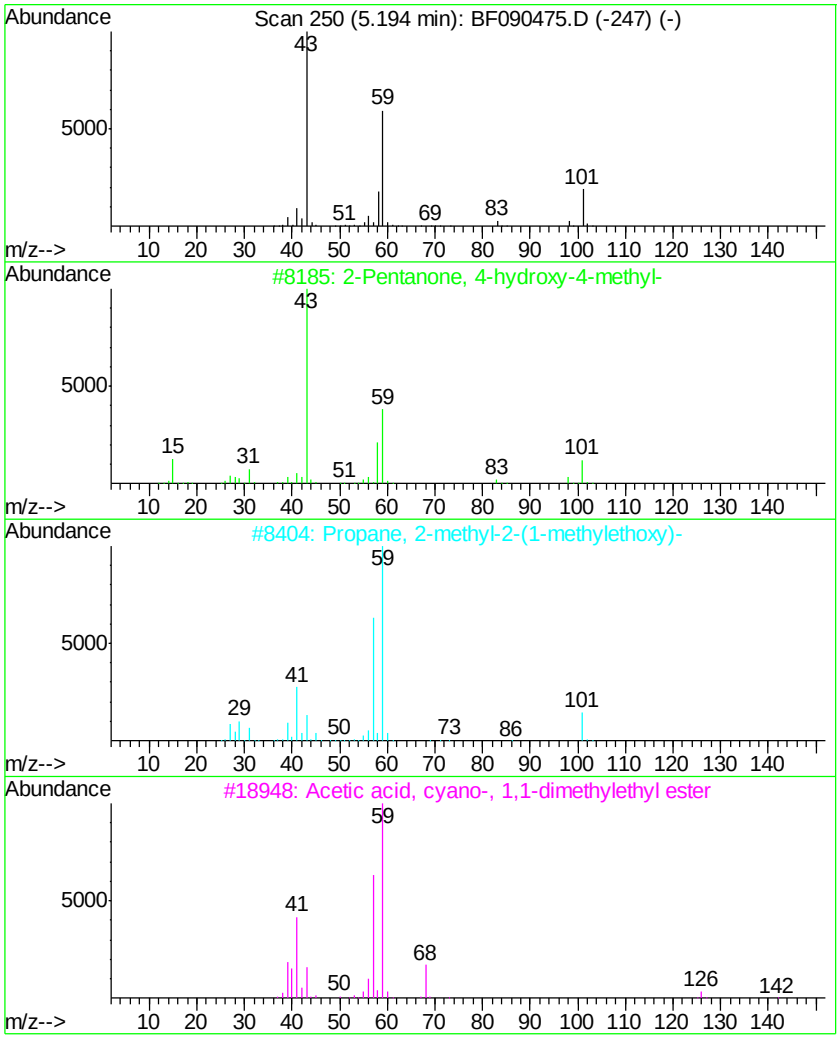
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

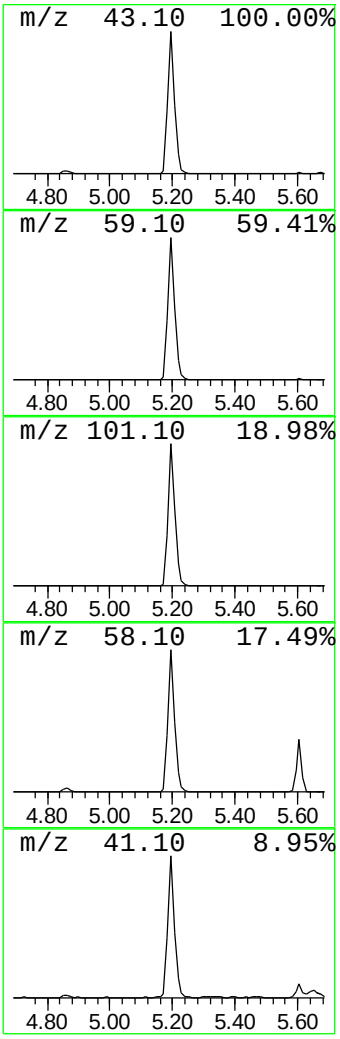
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	23.64 ng	1901190	1,4-Dichlorobenzene-d4	6.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

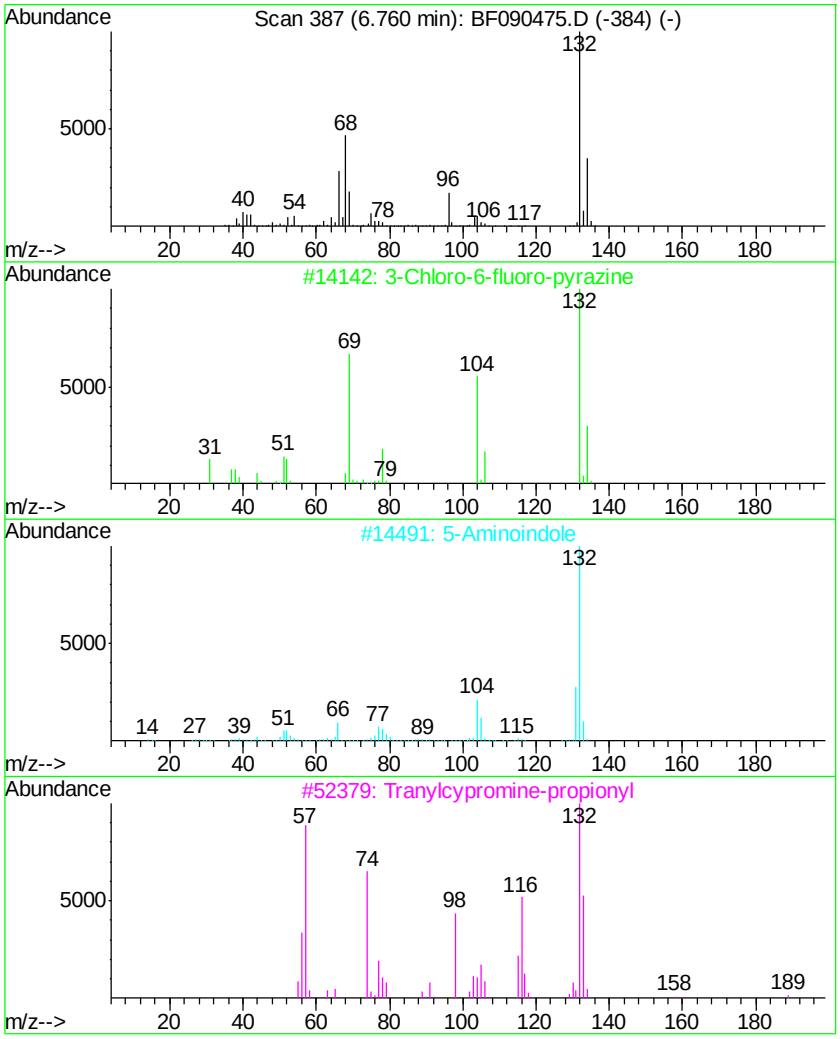
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

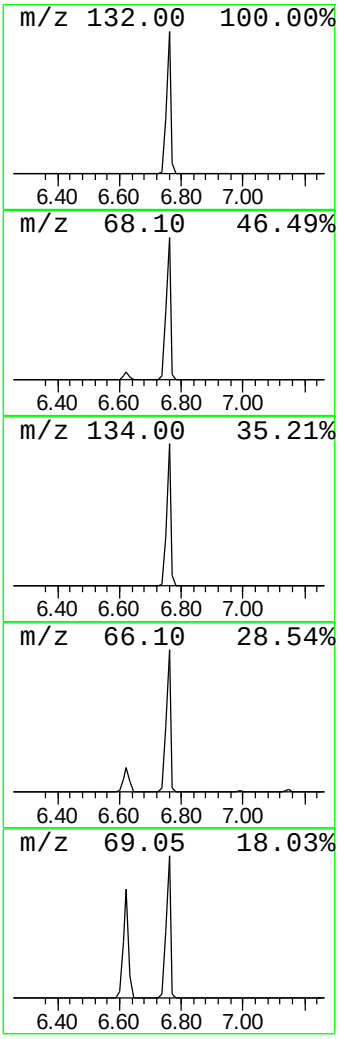
****

Peak Number 2 unknown6.76 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	87.91 ng	7069820	1,4-Dichlorobenzene-d4	6.99

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	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

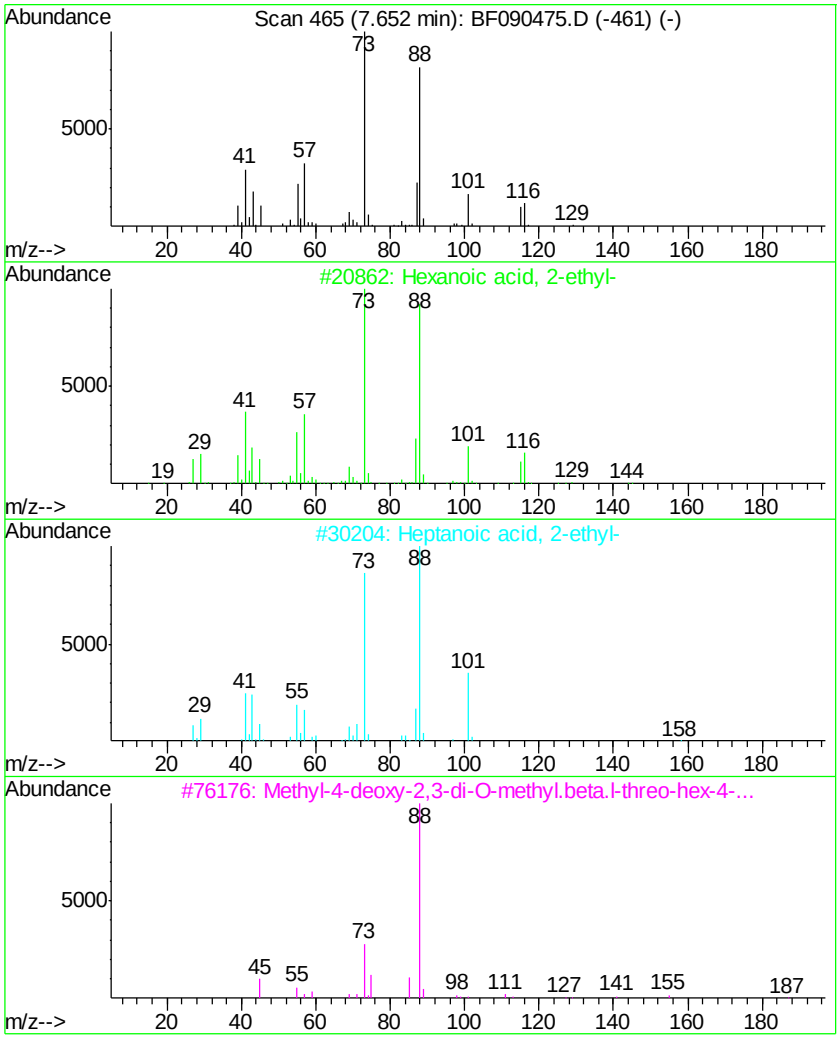
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

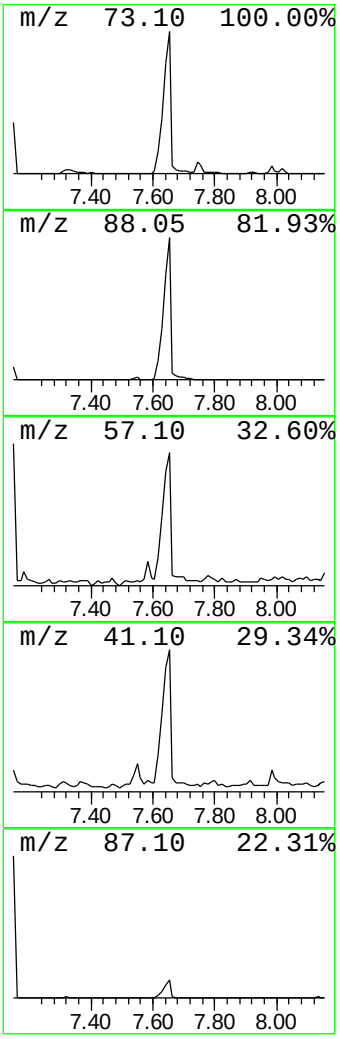
****

Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	3.05 ng	324886	Naphthalene-d8	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	59
3	Methyl-4-deoxy-2,3-di-O-methyl.b...	218	C9H14O6	1000312-09-9	53
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
5	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	40





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

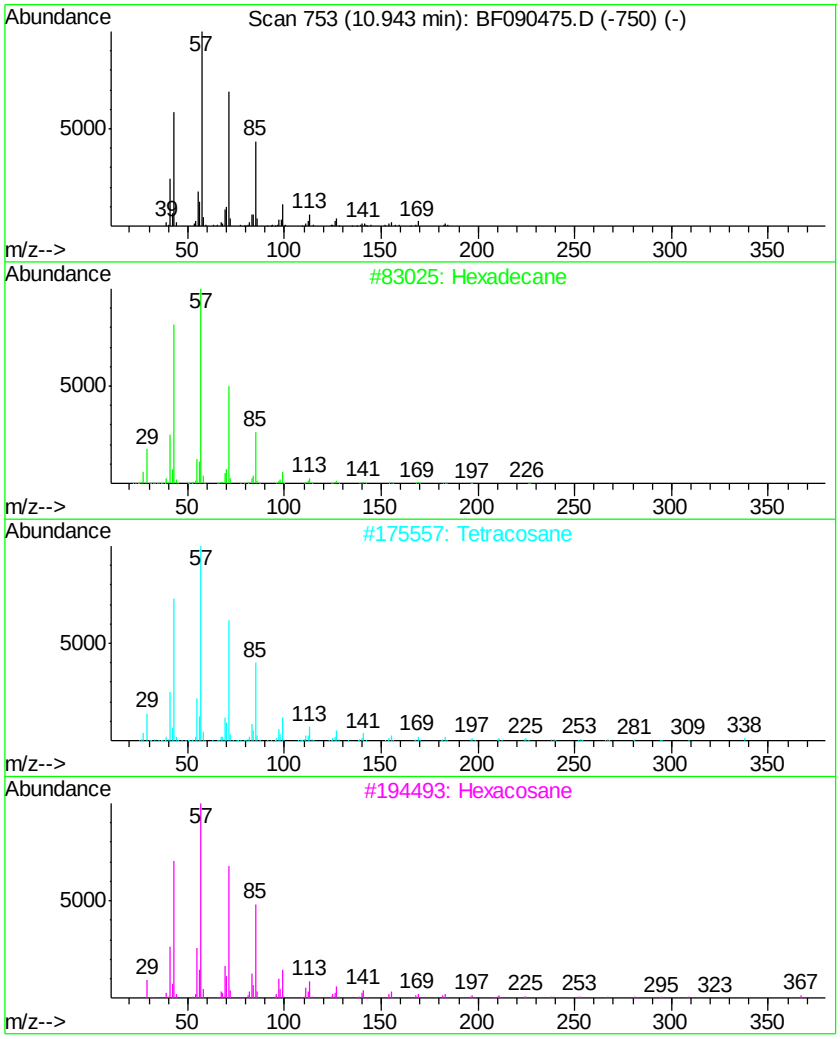
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

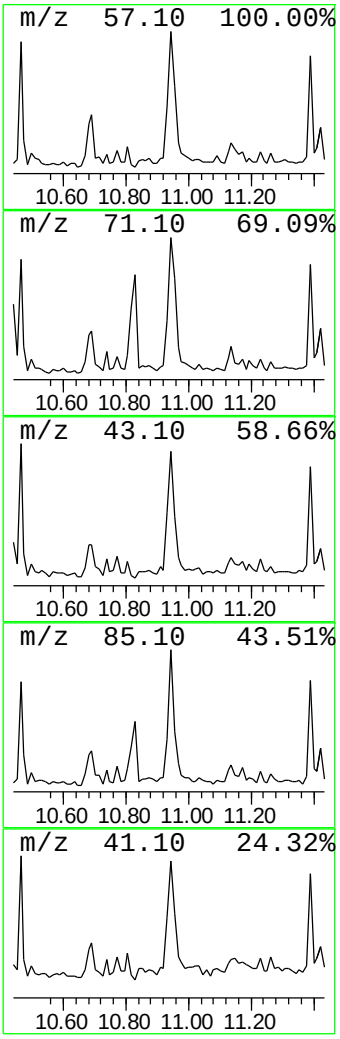
****

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.94	2.94 ng	342969	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	86
5	Dodecane, 4-methyl-	184	C13H28	006117-97-1	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

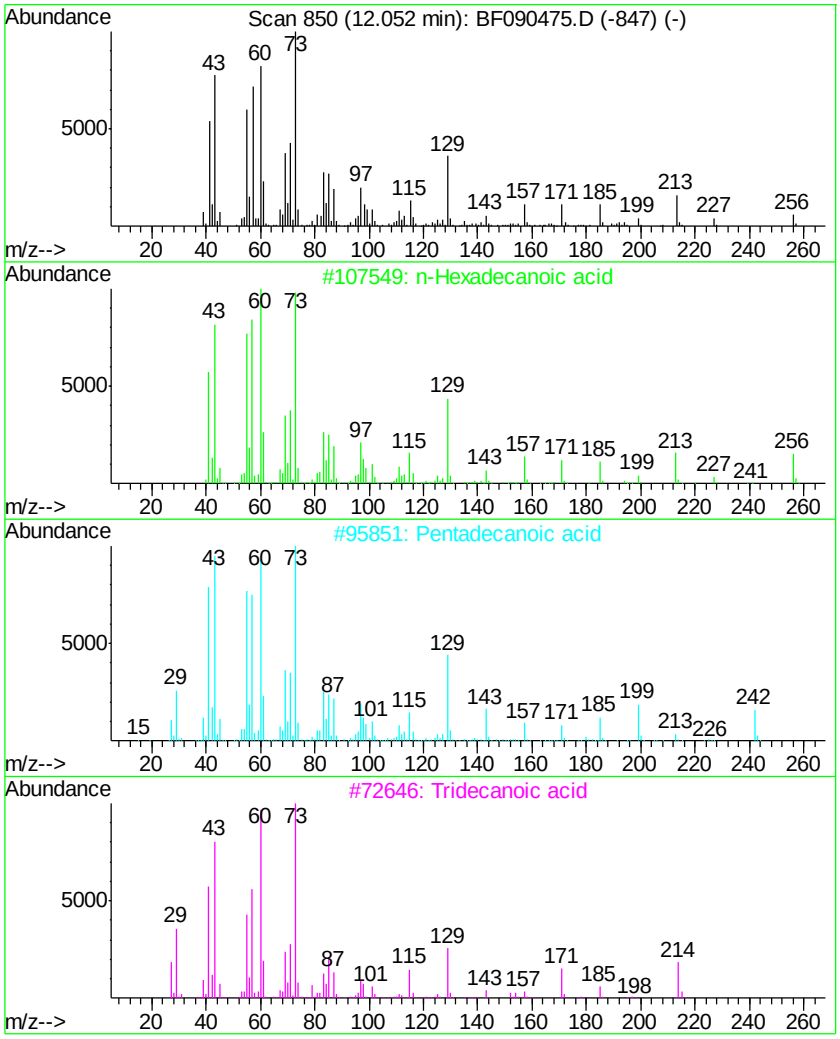
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

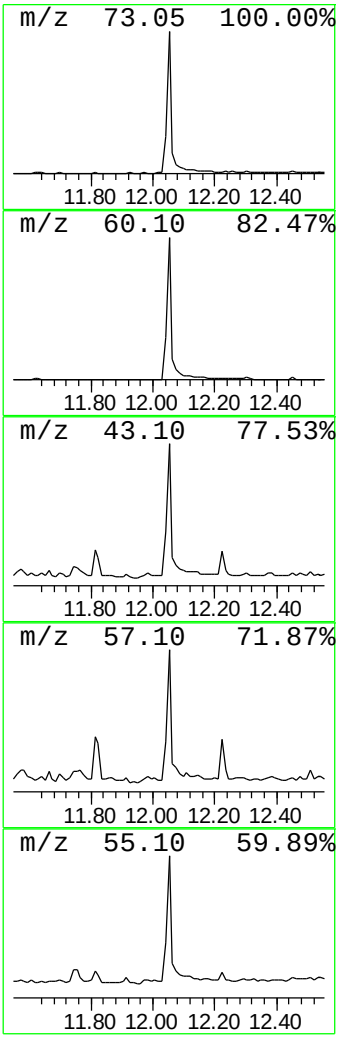
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	4.29 ng	501146	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

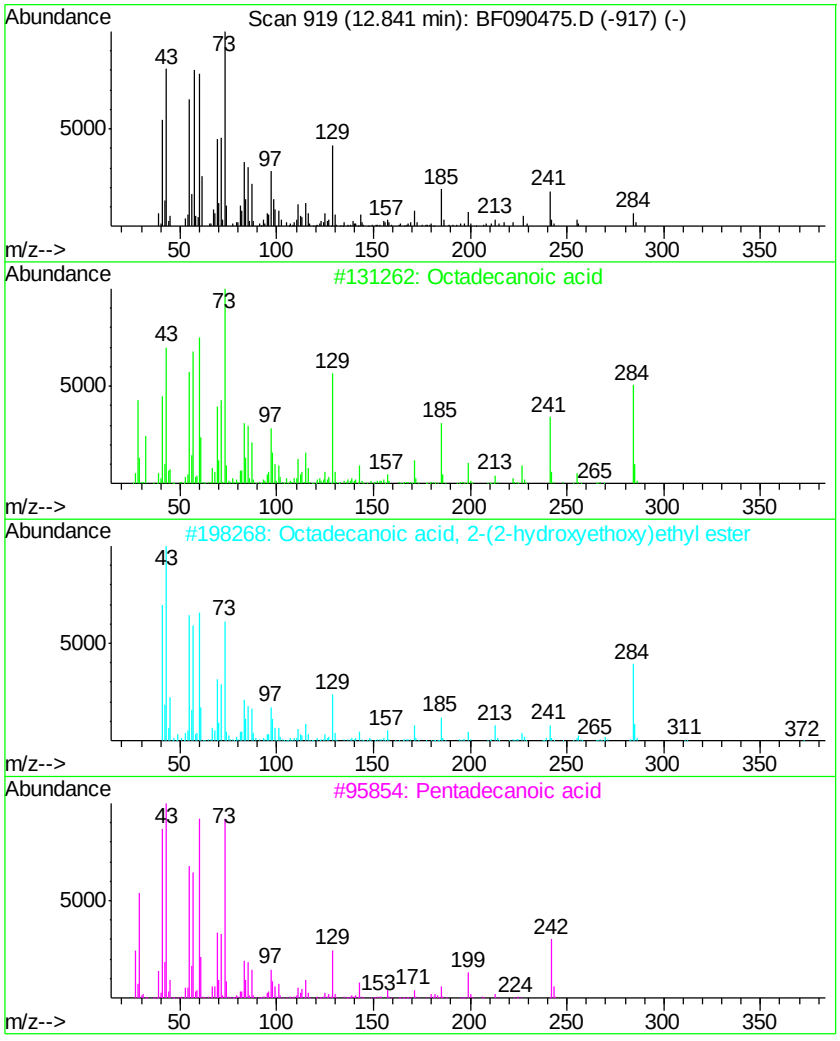
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

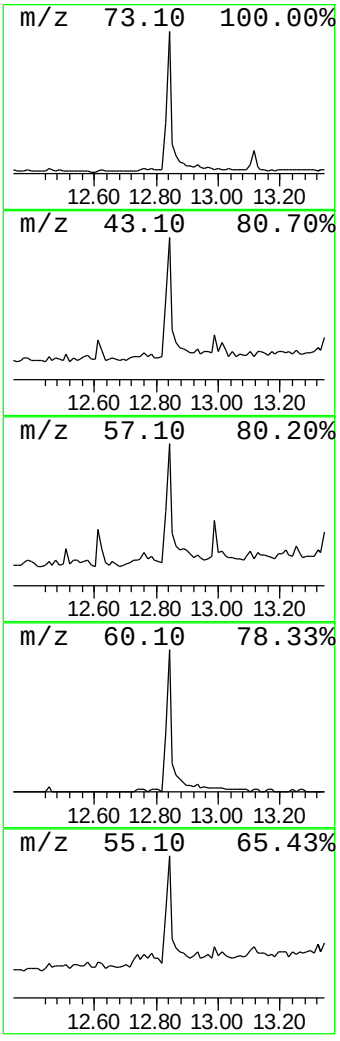
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	3.09 ng	360859	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

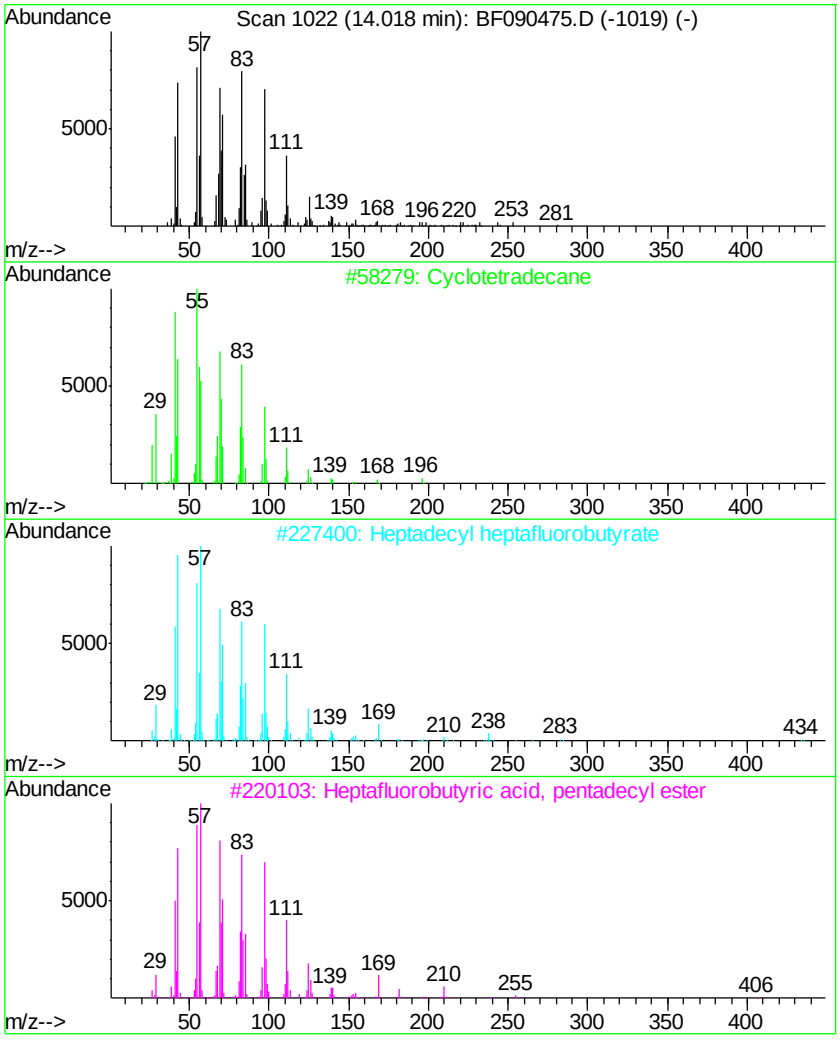
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

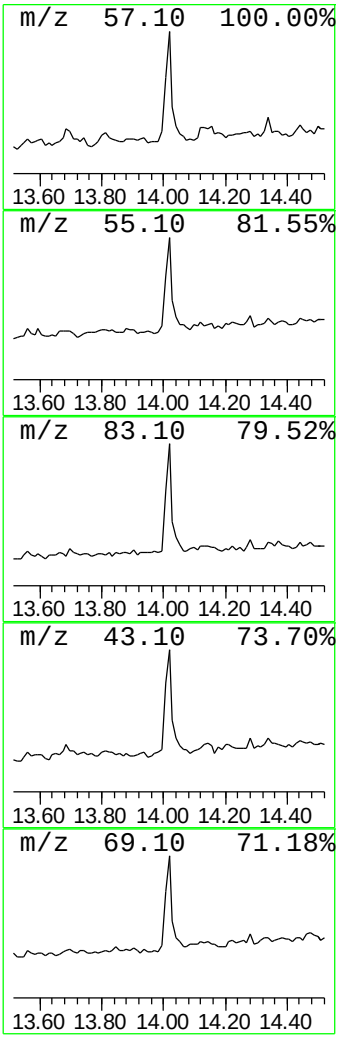
****

Peak Number 8 Cyclotetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	4.54 ng	313497	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	1-Docosene	308	C22H44	001599-67-3	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

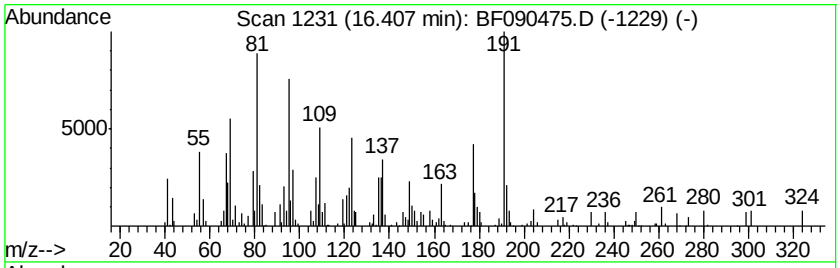
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

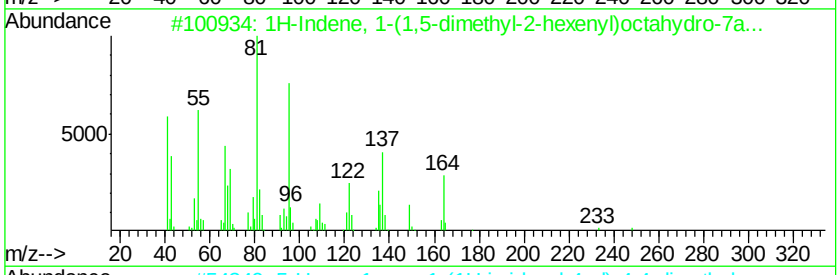
****

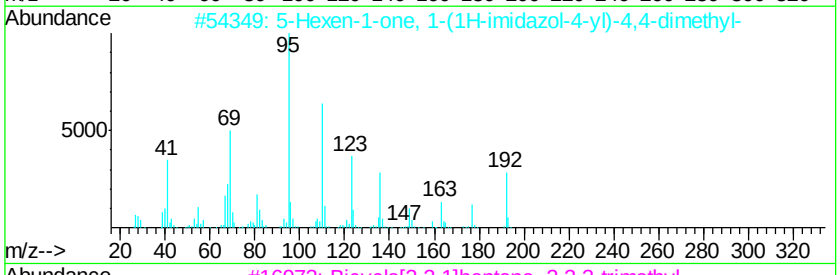
Peak Number 9 unknown16.41 Concentration Rank 9

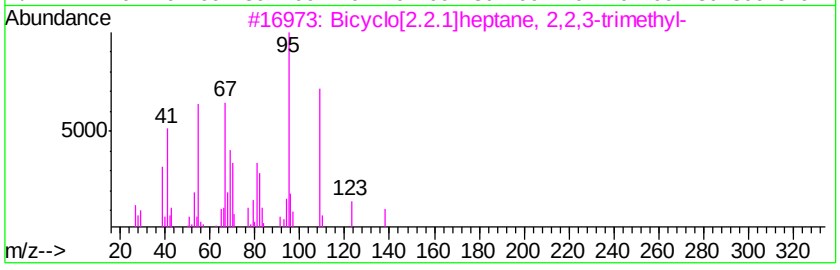
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	2.90 ng	172130	Perylene-d12	15.68

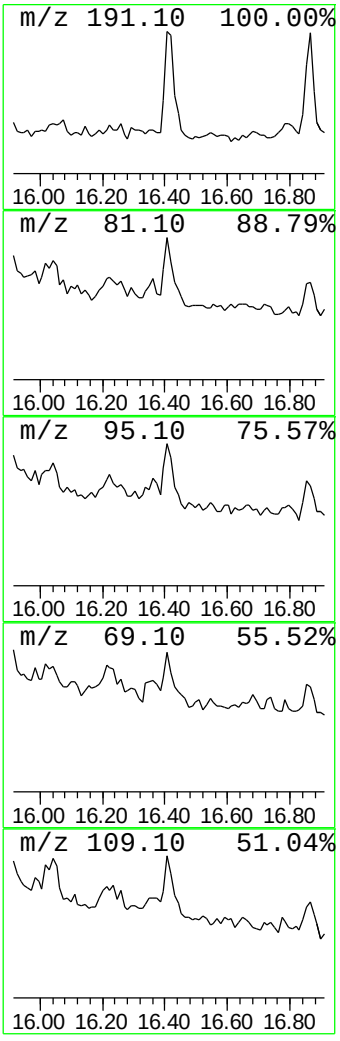
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 1-(1,5-dimethyl-2-hex...	248	C18H32	054411-95-9	35
2	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	35
3	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	35
4	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	27
5	1,10-Dimethyl-2-methylene-trans-...	178	C13H22	1000103-97-8	25











Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090475.D
Acq On : 8 Oct 2016 8:44
Operator : UM/SJ
Sample : H5136-11
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100516-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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
2-Pentanone, 4-hy...	5.19	23.6	ng	1901190	1	6.99	1608420	20.0
unknown6.76	6.76	87.9	ng	7069820	1	6.99	1608420	20.0
Hexanoic acid, 2-...	7.65	3.0	ng	324886	2	8.27	2129190	20.0
Hexadecane	10.94	2.9	ng	342969	4	11.53	2337000	20.0
n-Hexadecanoic acid	12.05	4.3	ng	501146	4	11.53	2337000	20.0
Octadecanoic acid	12.84	3.1	ng	360859	4	11.53	2337000	20.0
Cyclotetradecane	14.02	4.5	ng	313497	5	14.17	1380710	20.0
unknown16.41	16.41	2.9	ng	172130	6	15.68	1185720	20.0