LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090296.D
Acq On : 29 Sep 2016 18:22
Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

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-BF092016.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	1.644	3	5	20	rVB	313648	697797	17.58%	1.793%
2	4.547	256	259	275	rVB	391049	753885	19.00%	1.937%
3	5.027	298	301	303	rBV	2894429	3435293	86.57%	8.827%
4	6.125	394	397	400	rBV	2343904	3942306	99.34%	10.130%
5	6.227	404	406	409	rVB	2662277	3496865	88.12%	8.985%
6	6.456	424	426	429	rBV	654076	752325	18.96%	1.933%
7	6.616	437	440	443	rBV	2624646	2636893	66.45%	6.776%
8	7.039	474	477	479	rBV	2087018	2251669	56.74%	5.786%
9	7.748	537	539	542	rBV	1027657	998645	25.17%	2.566%
10	8.833	631	634	637	rBV	2850232	3968334	100.00%	10.197%
11	9.233	667	669	672	rVV	758908	1066318	26.87%	2.740%
12	9.359	675	680	682	rBV	55170	60833	1.53%	0.156%
13	9.462	687	689	690	rBV	53961	45105	1.14%	0.116%
14	9.496	690	692	694	rBV	1297130	1105366	27.85%	2.840%
15	9.965	729	733	734	rVB	83978	108241	2.73%	0.278%
16	10.182	748	752	753	rBV2	46405	74086	1.87%	0.190%
17	10.285	758	761	764	rBV	1953820	2133236	53.76%	5.482%
18	10.434	770	774	777	rBV	126286	189605	4.78%	0.487%
19	10.879	811	813	814	rBV2	63345	68142	1.72%	0.175%
20	10.971	818	821	822	rBV	1041091	1008484	25.41%	2.591%
21	10.994	822	823	824	rVV	163651	118607	2.99%	0.305%
22	11.039	824	827	832	rVB2	62269	98224	2.48%	0.252%
23	11.234	841	844	846	rBV2	113091	163633	4.12%	0.420%
24	11.302	848	850	852	rVB	43630	45377	1.14%	0.117%
25	11.462	862	864	866	rBV2	35796	65933	1.66%	0.169%
26	11.496	866	867	869	rVV	54204	48375	1.22%	0.124%
27	11.542	869	871	873	rVV2	263146	290570	7.32%	0.747%
28	11.577	873	874	880	rVB	85582	114501	2.89%	0.294%
29	11.782	888	892	896	rVB3	53926	93626	2.36%	0.241%
30	11.919	901	904	905	rBV	51309	54762	1.38%	0.141%
31	12.011	911	912	914	rBV	32916	45937	1.16%	0.118%
32	12.091	918	919	924	rVB2	36953	46807	1.18%	0.120%
33	12.171	924	926	928	rBV	413479	425445	10.72%	1.093%
34	12.319	936	939	942	rBV3	83255	136654	3.44%	0.351%

LSC Area Percent Report

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Acq On : 29 Sep 2016 18:22
Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

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-BF092016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.388	942	945	949	rBV	390663	499235	12.58%	1.283%
36	12.559	957	960	962	rBV	2654014	2705570	68.18%	6.952%
37	12.617	962	965	967	rVB2	34197	59732	1.51%	0.153%
38	12.719	972	974	976	rVB	58755	92971	2.34%	0.239%
39	12.788	978	980	982	rBV	85930	113200	2.85%	0.291%
40	12.822	982	983	987	rVB2	73556	91043	2.29%	0.234%
41	13.108	1006	1008	1009	rBV2	42684	50325	1.27%	0.129%
42	13.337	1026	1028	1029	rBV	38767	54906	1.38%	0.141%
43	13.474	1038	1040	1044	rBV	367718	474121	11.95%	1.218%
44	13.588	1047	1050	1054	rBV2	724268	1225614	30.88%	3.149%
45	13.794	1066	1068	1073	rBV3	63859	100265	2.53%	0.258%
46	14.102	1093	1095	1098	rBV3	295359	366468	9.23%	0.942%
47	14.457	1123	1126	1128	rBV	259897	265848	6.70%	0.683%
48	14.571	1134	1136	1140	rBV	268019	472155	11.90%	1.213%
49	14.811	1155	1157	1159	rBV	157472	175812	4.43%	0.452%
50	14.857	1159	1161	1164	rVV	172827	215671	5.43%	0.554%
51	14.914	1164	1166	1171	rVB2	521195	644824	16.25%	1.657%
52	15.143	1184	1186	1188	rBV	80786	110114	2.77%	0.283%
53	15.360	1203	1205	1208	rVB2	119733	165014	4.16%	0.424%
54	15.931	1253	1255	1259	rVB2	116275	211071	5.32%	0.542%
55	16.057	1264	1266	1271	rVB2	80965	154103	3.88%	0.396%
56	16.400	1294	1296	1300	rVB	67776	126977	3.20%	0.326%

Sum of corrected areas: 38916918

LSC Report - Integrated Chromatogram

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Data File : BF090296.D
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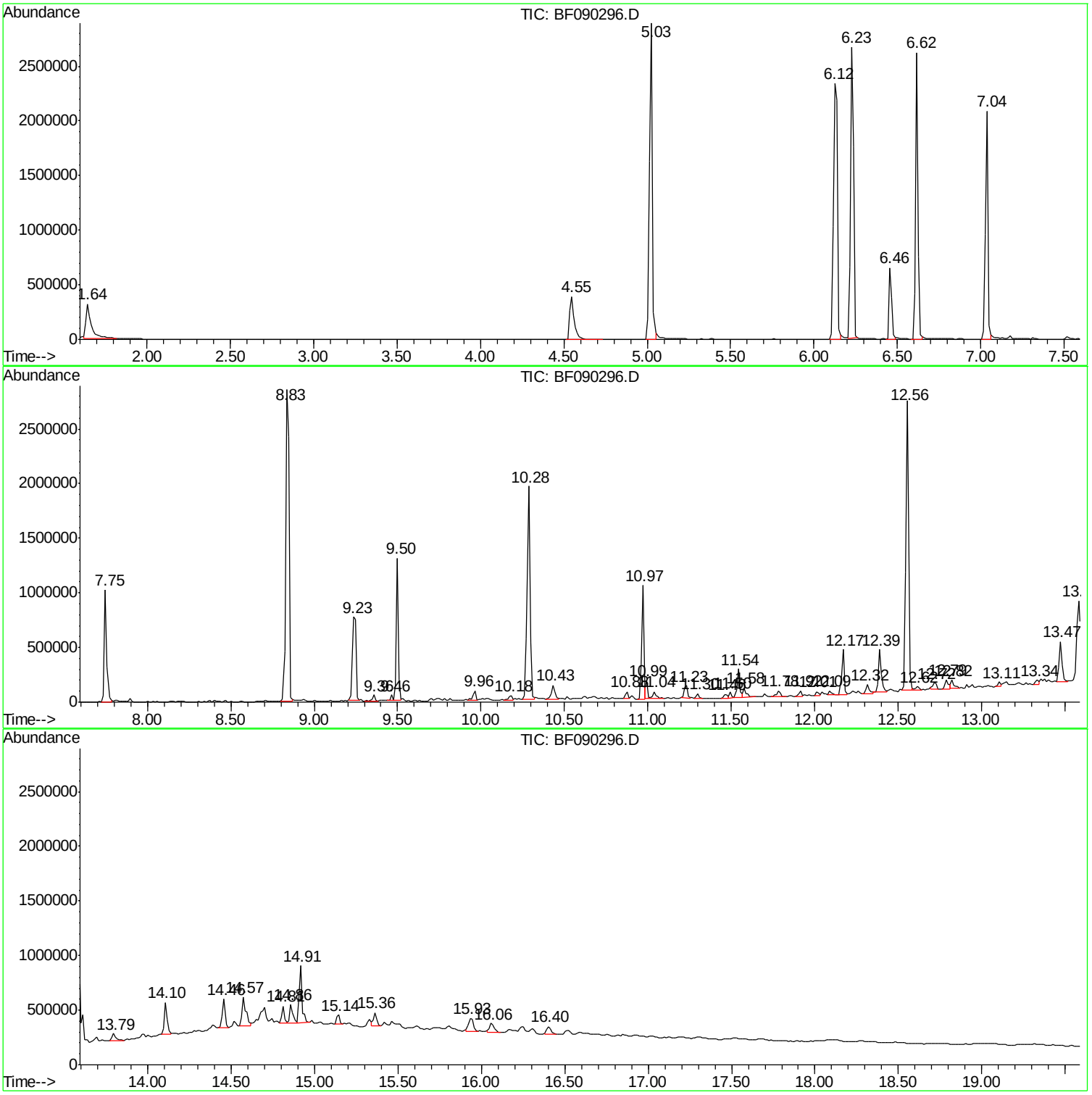
Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090296.D
Acq On : 29 Sep 2016 18:22
Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

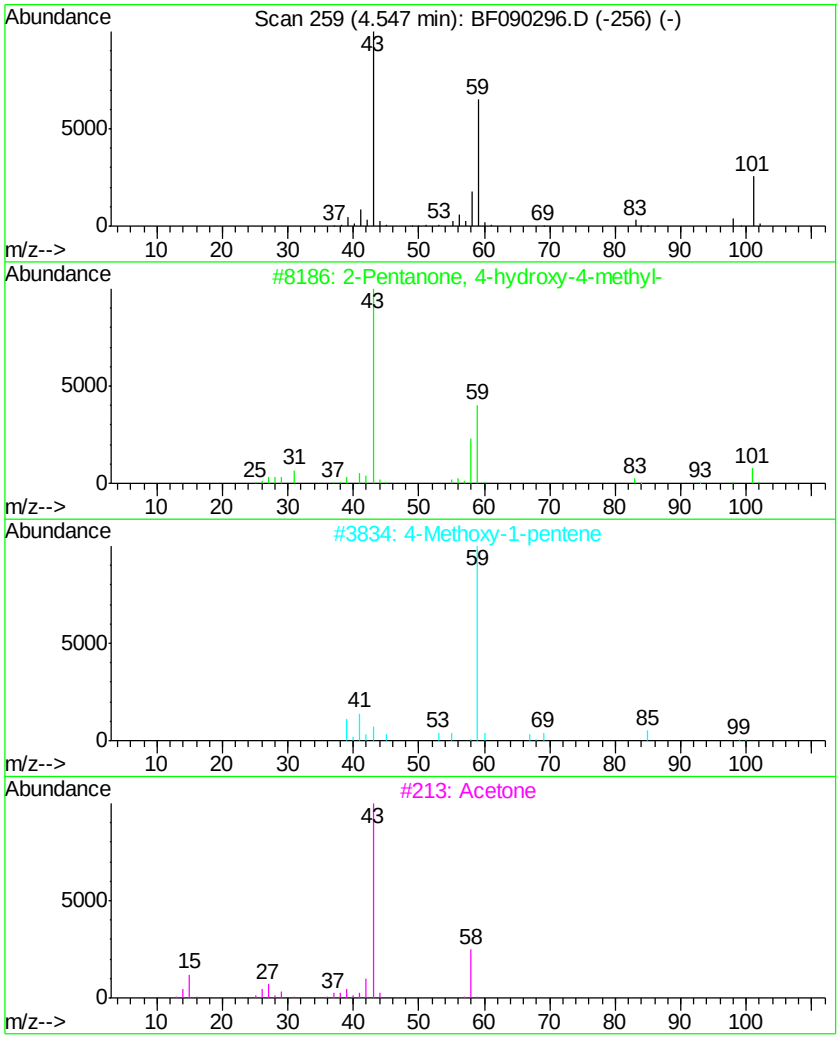
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

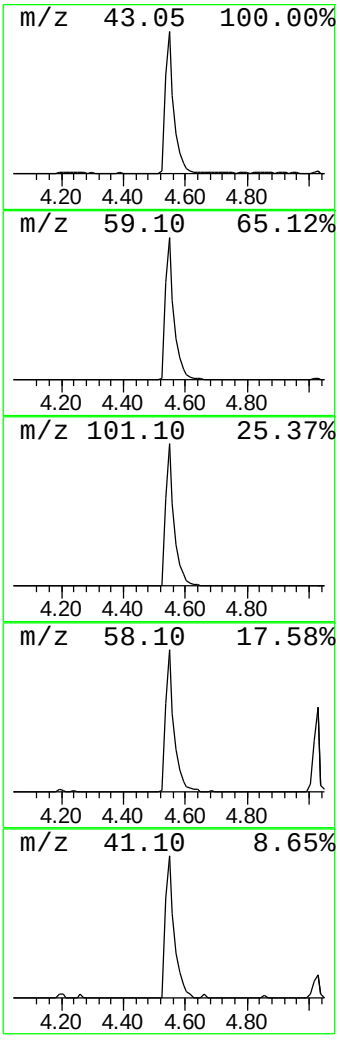
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	20.04 ng	753885	1,4-Dichlorobenzene-d4	6.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	17
3	Acetone	58	C3H6O	000067-64-1	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090296.D
Acq On : 29 Sep 2016 18:22
Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

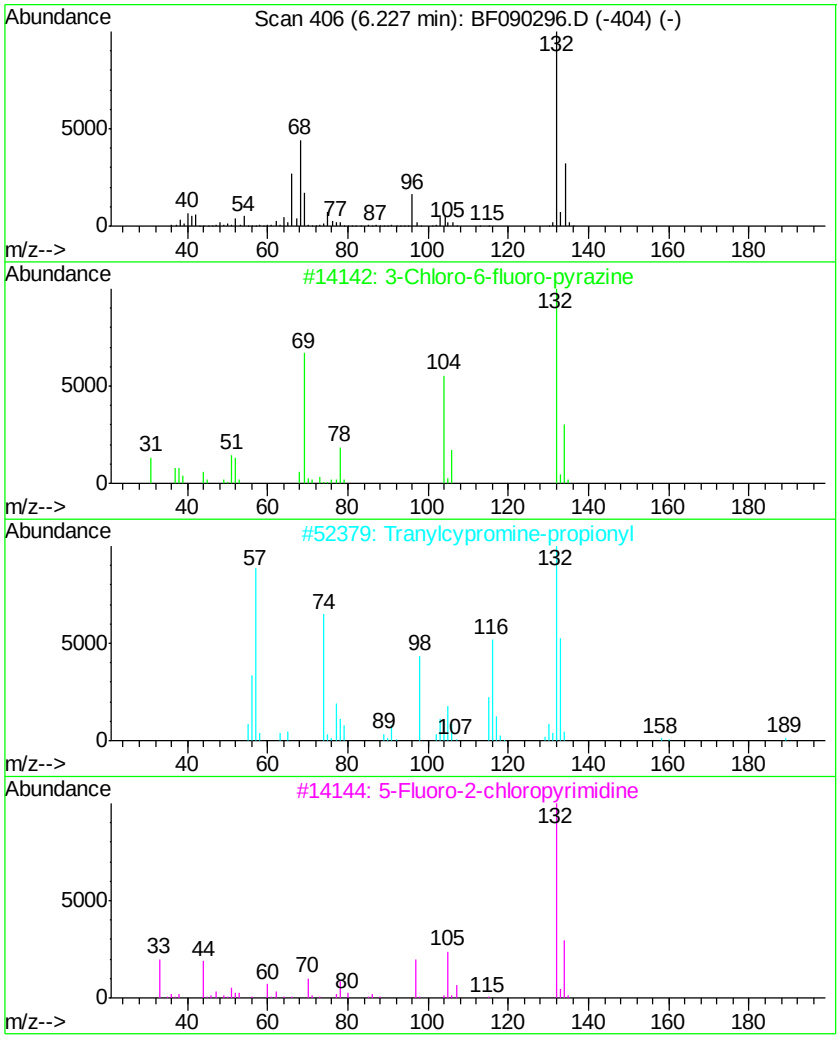
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

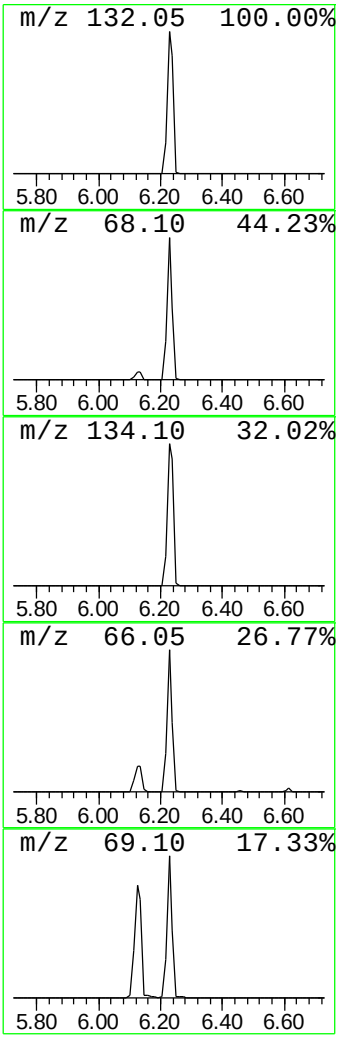
****

Peak Number 3 unknown6.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.23	92.96 ng	3496870	1,4-Dichlorobenzene-d4	6.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090296.D
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Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

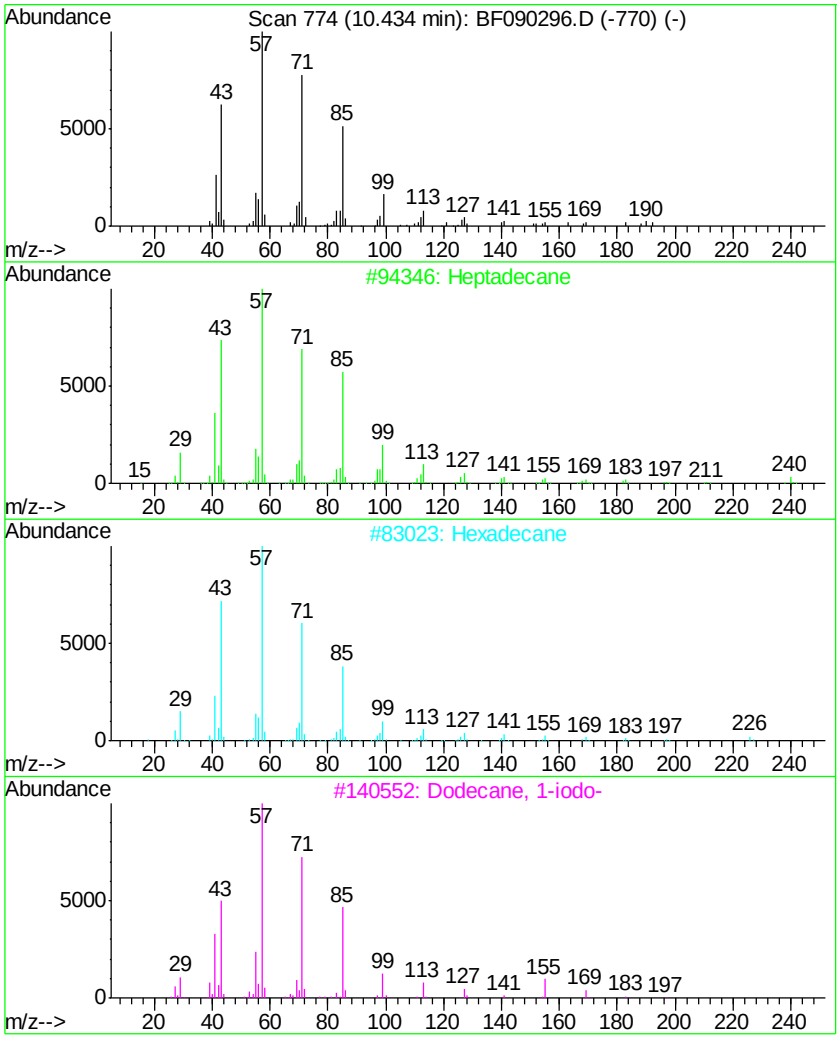
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

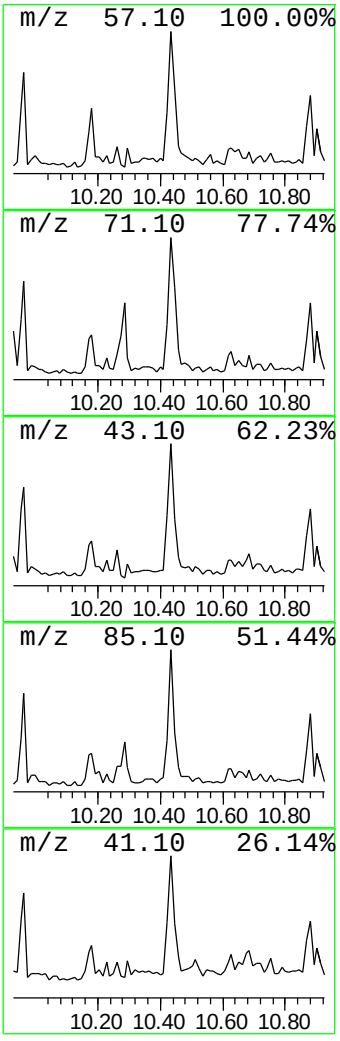
****

Peak Number 5 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	3.76 ng	189605	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

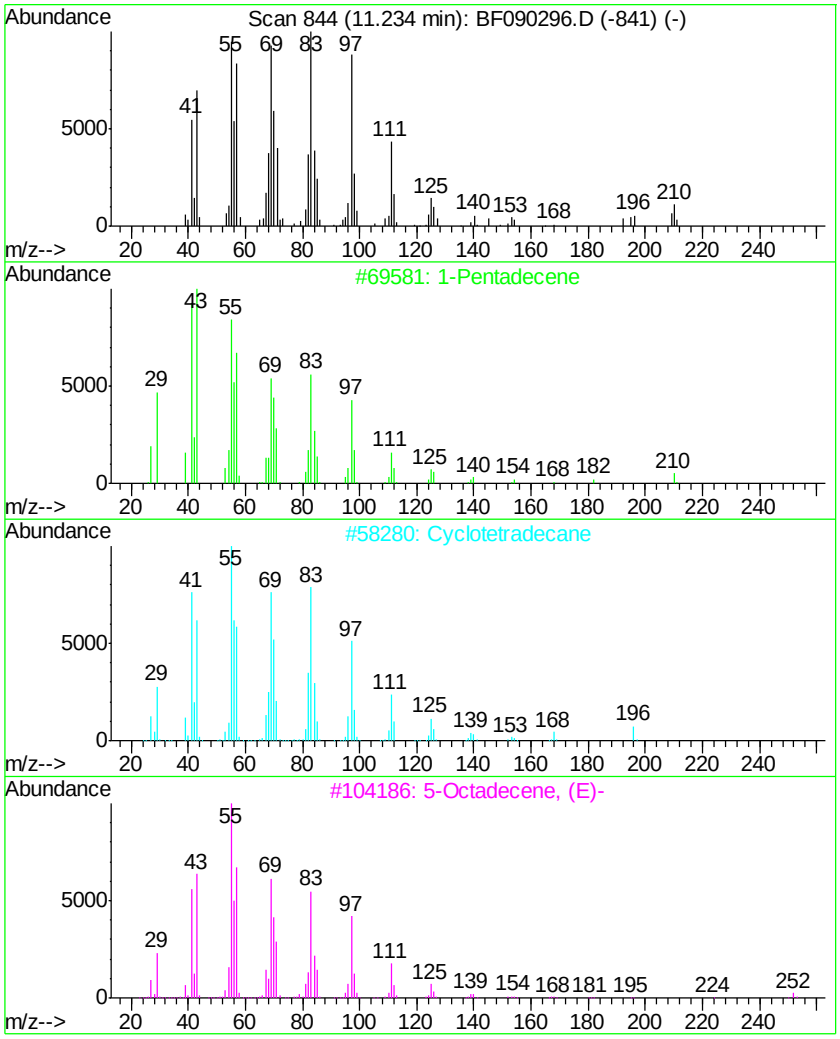
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

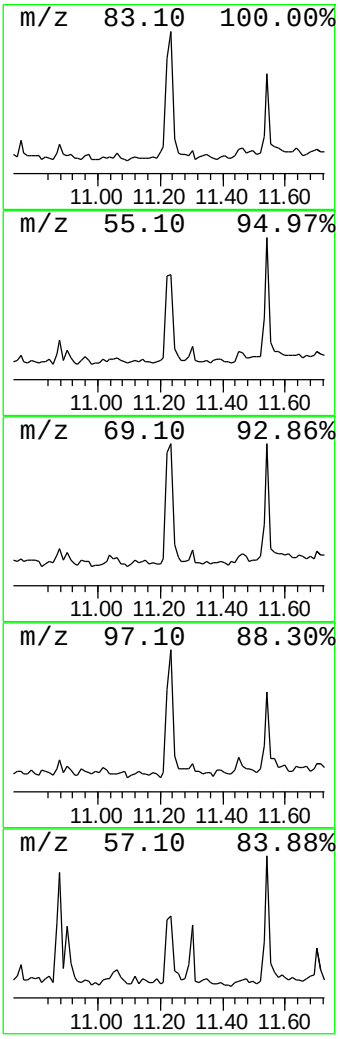
****

Peak Number 6 1-Pentadecene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.23	3.25 ng	163633	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecene	210	C15H30	013360-61-7	98
2	Cyclotetradecane	196	C14H28	000295-17-0	93
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
4	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91





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Sample : H4982-09
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Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

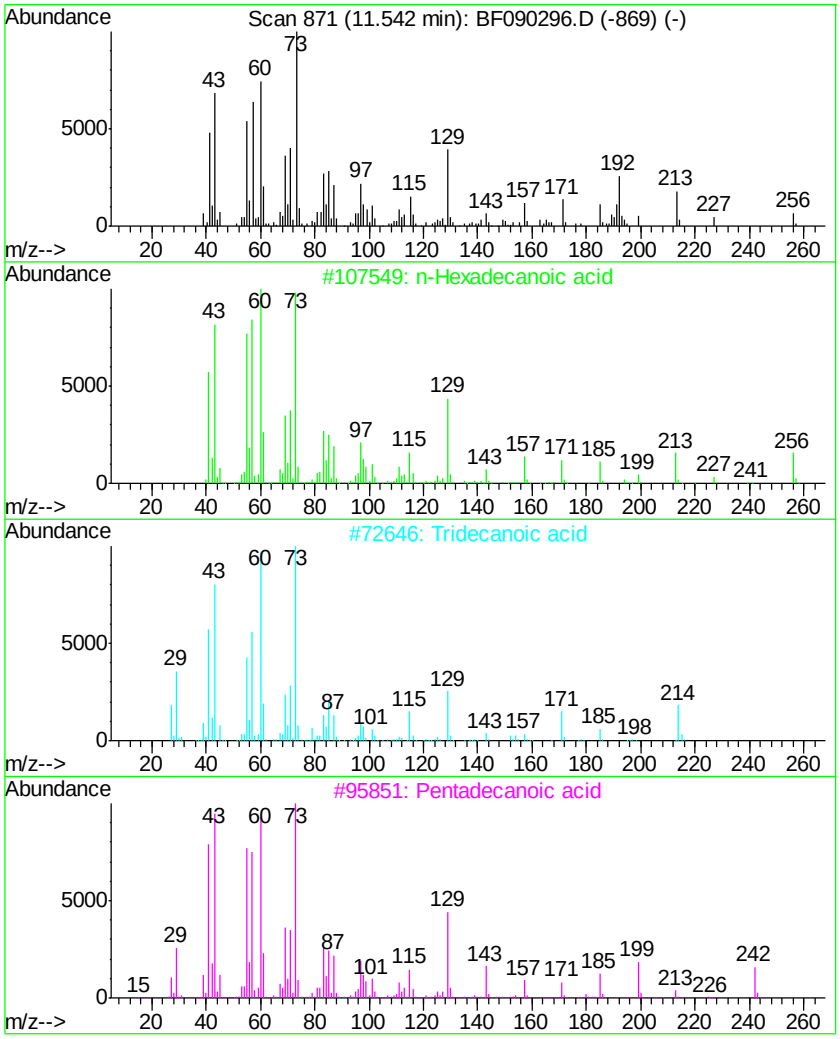
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

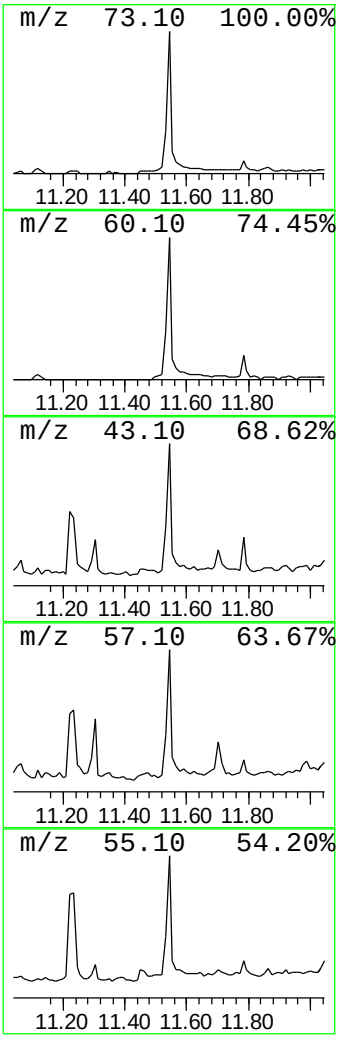
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	5.76 ng	290570	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	25





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Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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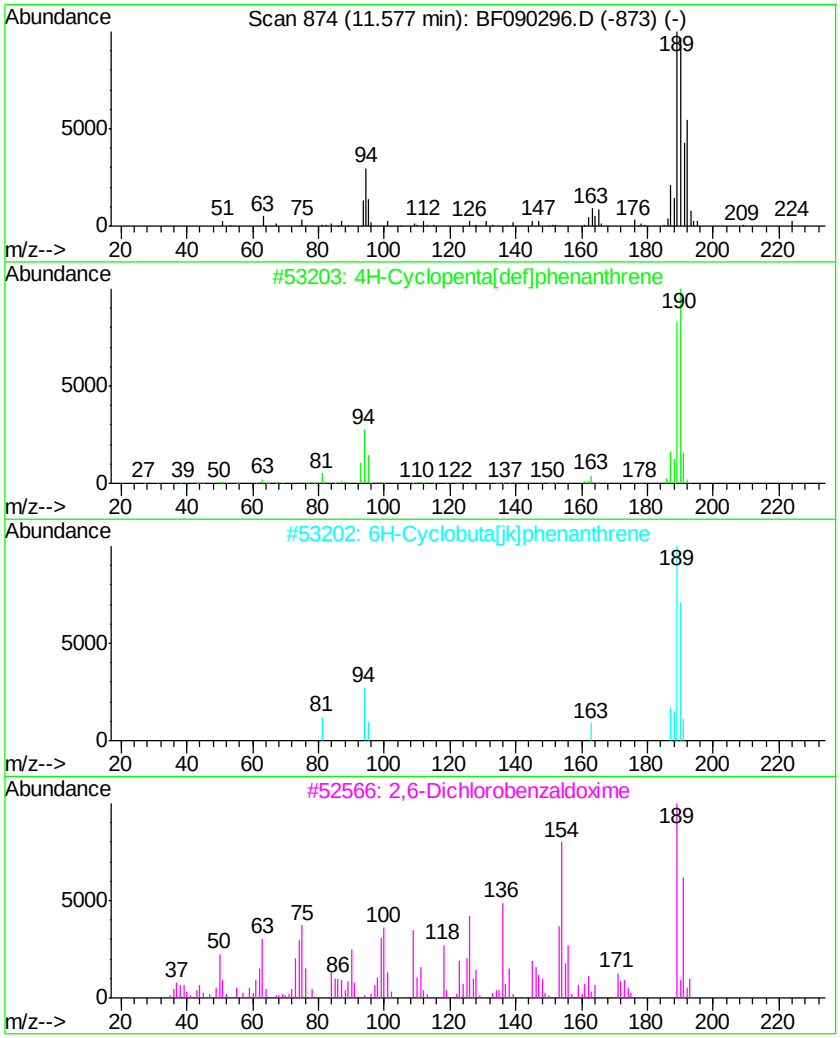
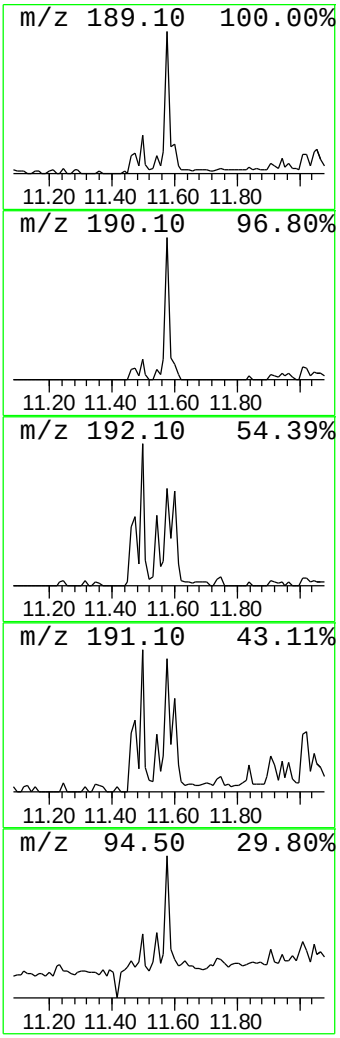
Peak Number 8 4H-Cyclopenta[def]phenanthrene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	2.27 ng	114501	Phenanthrene-d10	10.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	68
3	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	42
4	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40
5	5-Thiazolecarboxamide, 4-amino-2...	189	C5H7N3OS2	1000338-08-9	14





Library Search Compound Report

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Data File : BF090296.D
Acq On : 29 Sep 2016 18:22
Operator : UM/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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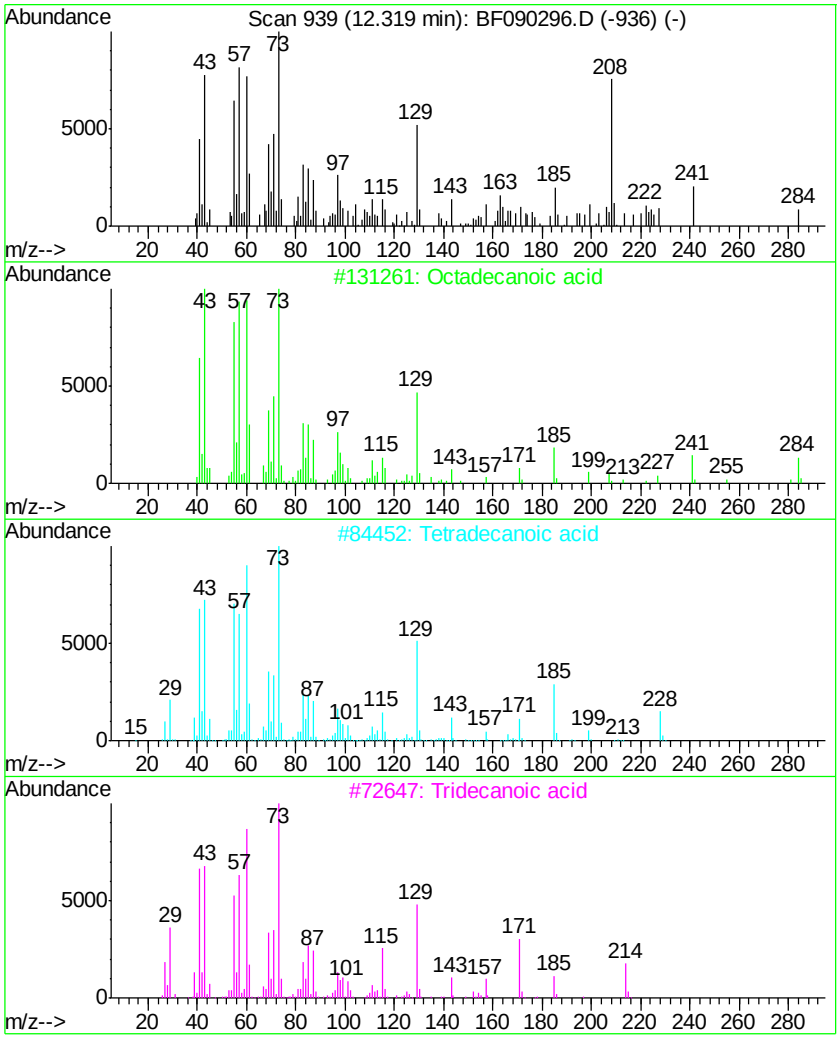
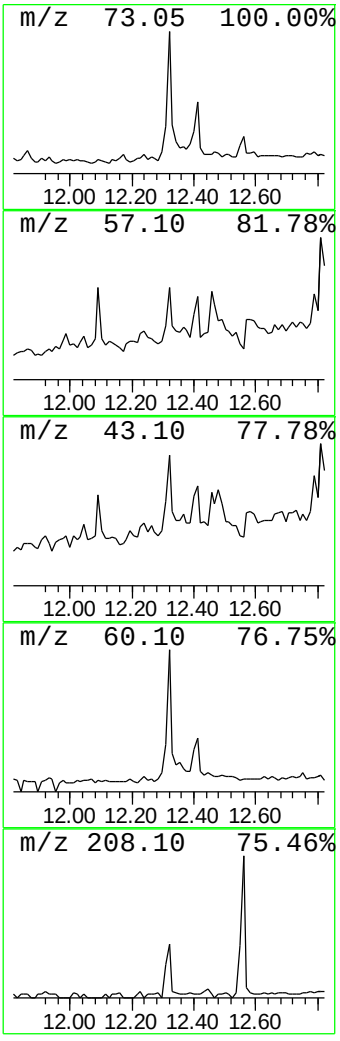
Peak Number 9 Octadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	2.23 ng	136654	Chrysene-d12	13.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
3	Tridecanoic acid	214	C13H26O2	000638-53-9	46
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092916\
Data File : BF090296.D
Acq On : 29 Sep 2016 18:22
Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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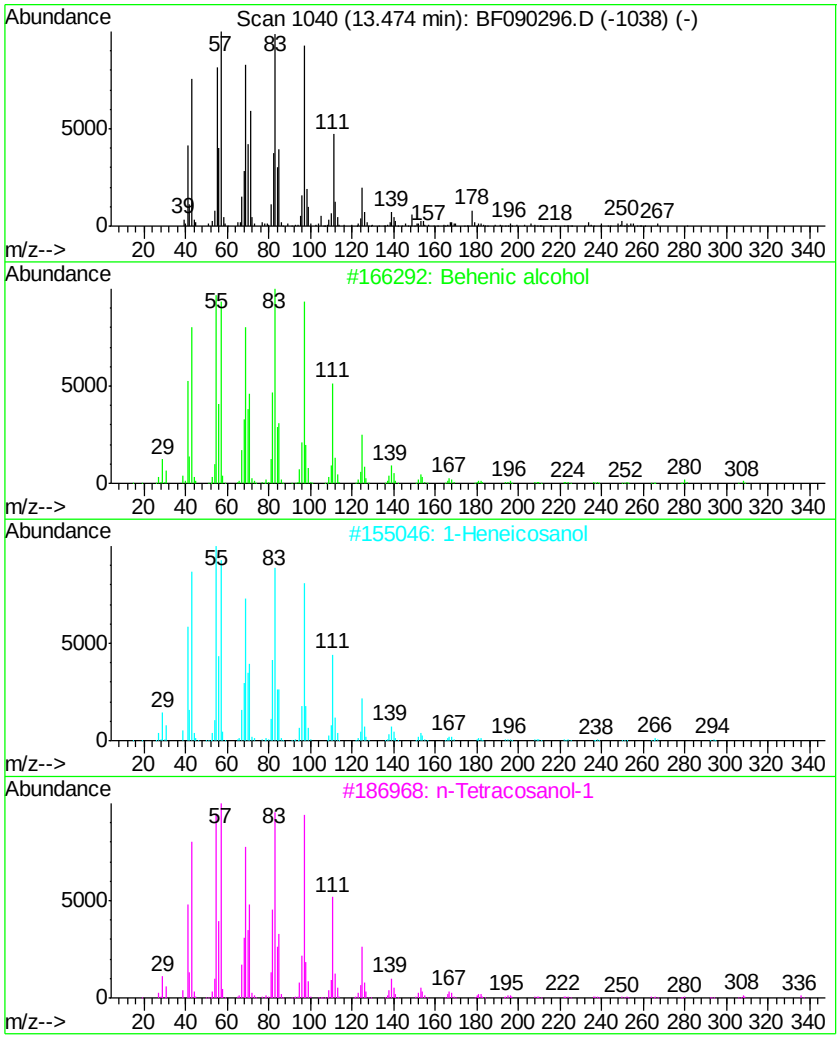
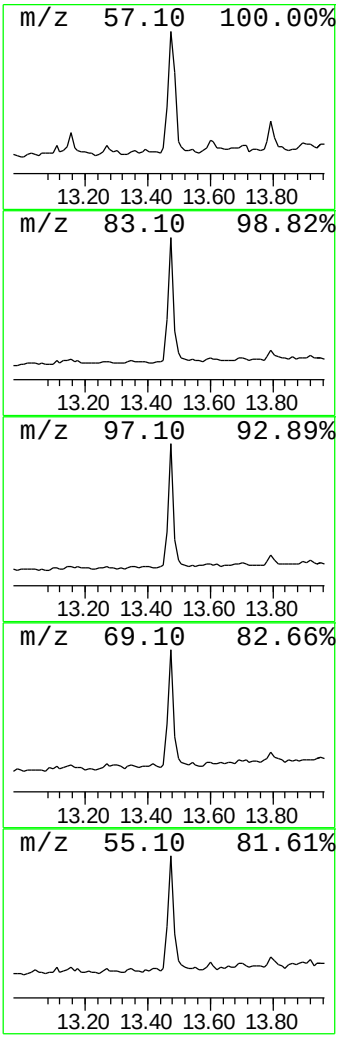
Peak Number 10 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	7.74 ng	474121	Chrysene-d12	13.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90





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Data File : BF090296.D
Acq On : 29 Sep 2016 18:22
Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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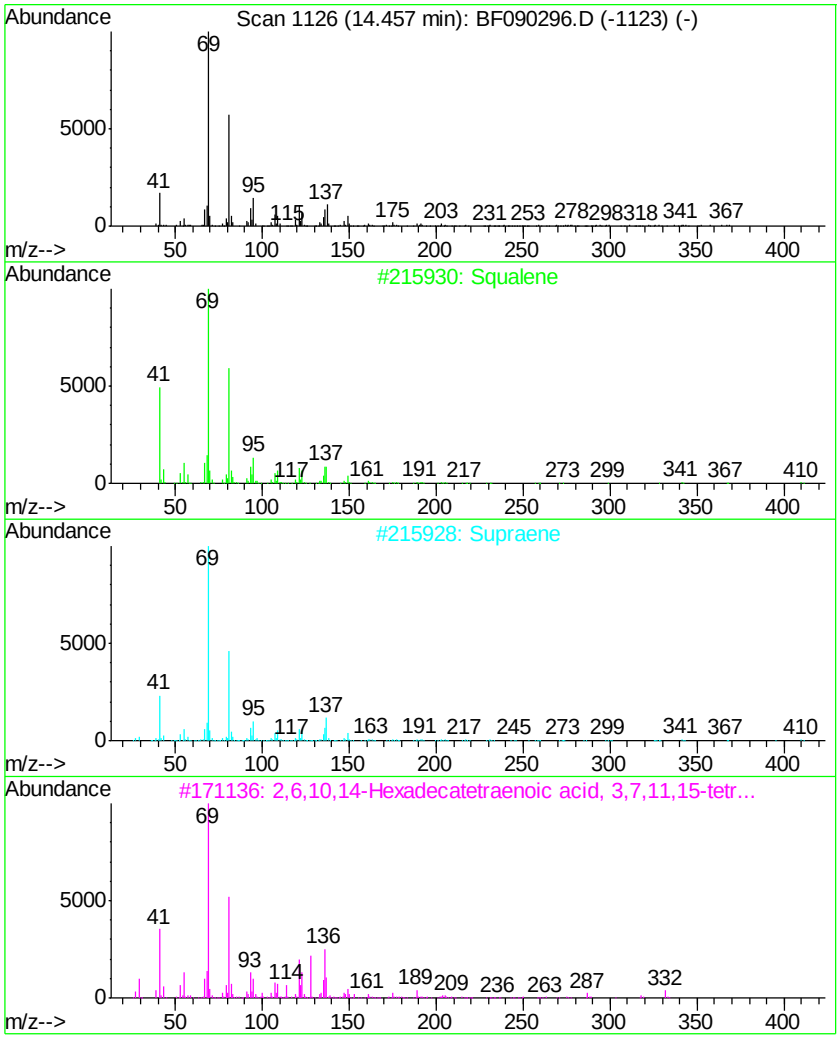
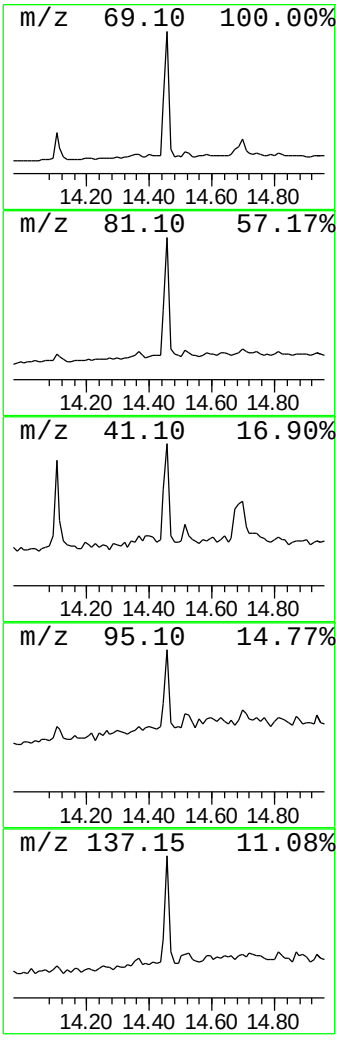
Peak Number 12 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	8.25 ng	265848	Perylene-d12	14.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	90
4	Diethylmalonic acid, monochlorid...	352	C10H13BrClF3O3	1000370-81-2	50
5	1,5-Heptadiene, 3,3-dimethyl-, (E)-	124	C9H16	067682-47-7	47





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Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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TIC Integration Parameters: LSCINT.P

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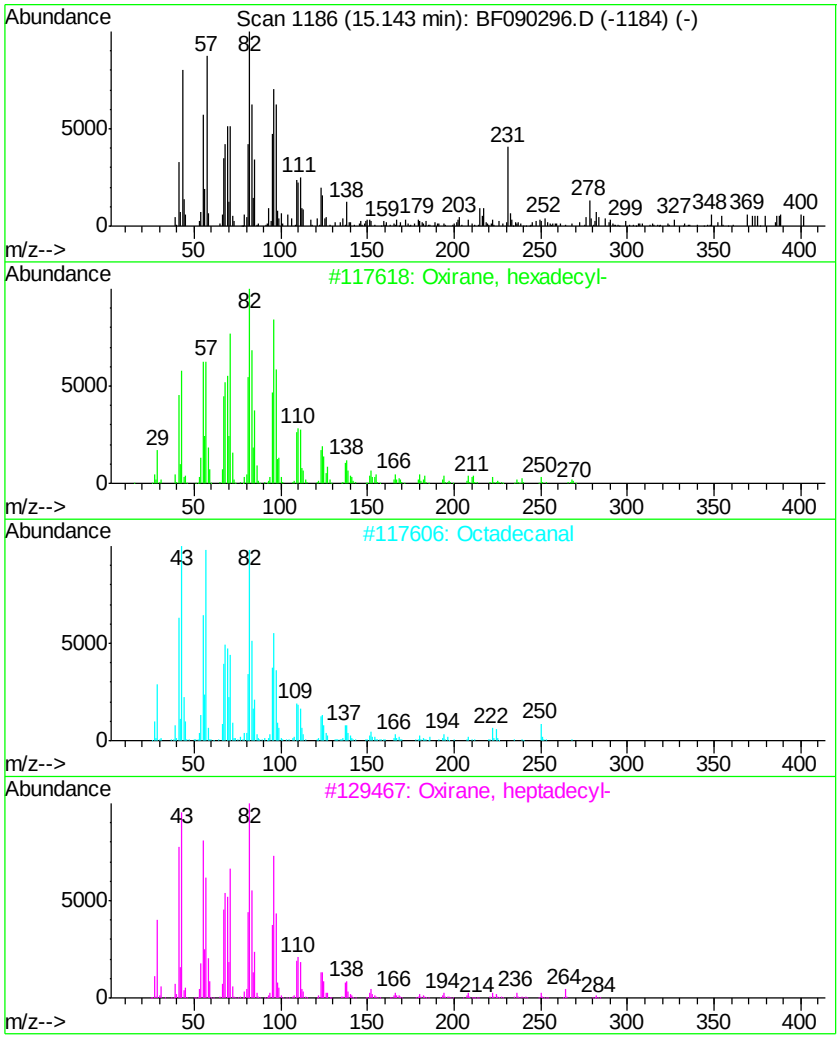
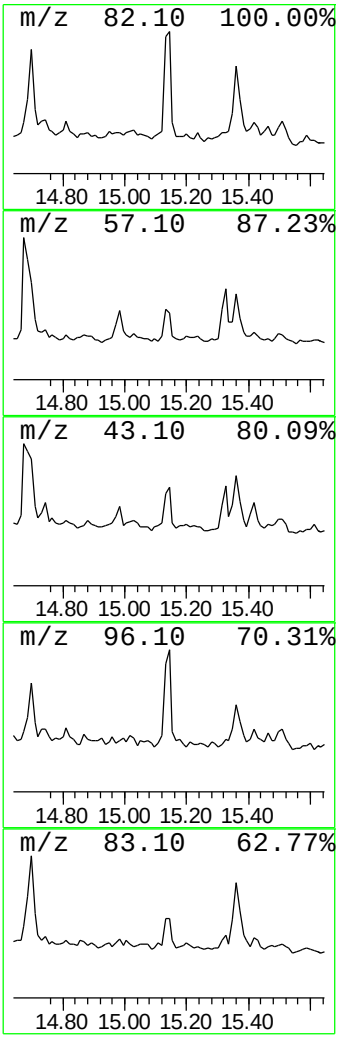
Peak Number 13 Oxirane, hexadecyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	3.42 ng	110114	Perylene-d12	14.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
2	Octadecanal	268	C18H36O	000638-66-4	83
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	81
4	Tetradecanal	212	C14H28O	000124-25-4	78
5	Bicyclo[10.8.0]eicosane, cis-	278	C20H38	1000155-82-2	78





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Data File : BF090296.D
Acq On : 29 Sep 2016 18:22
Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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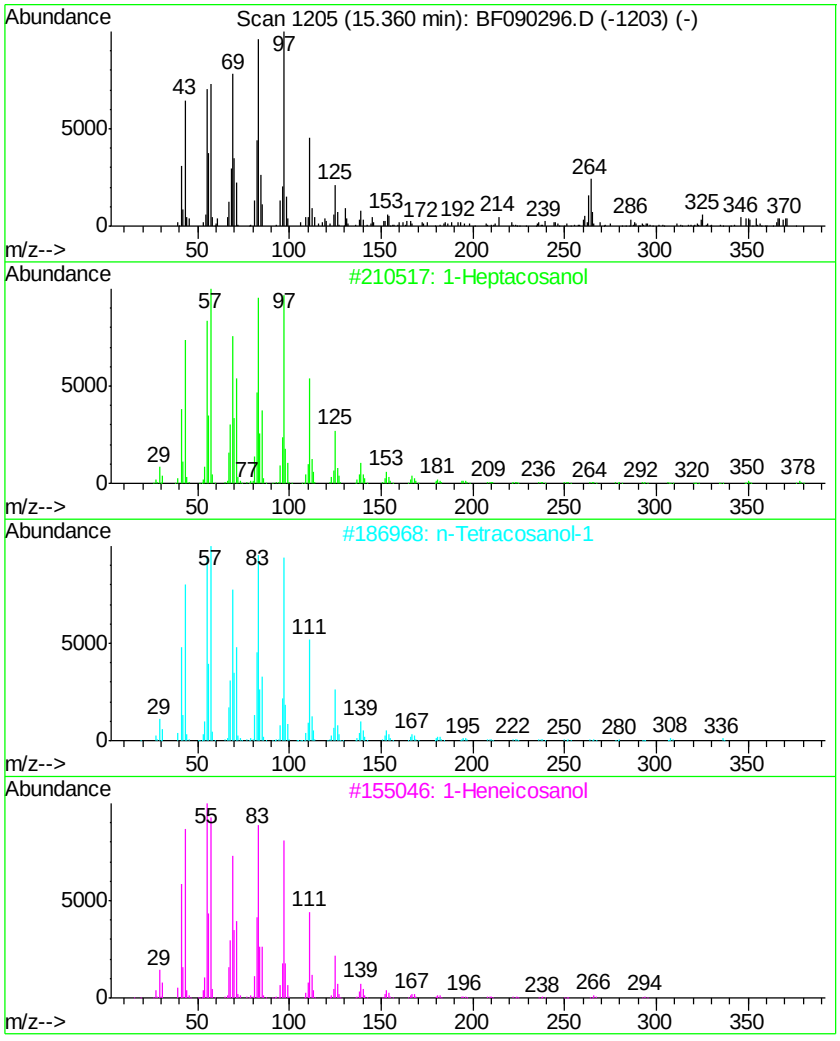
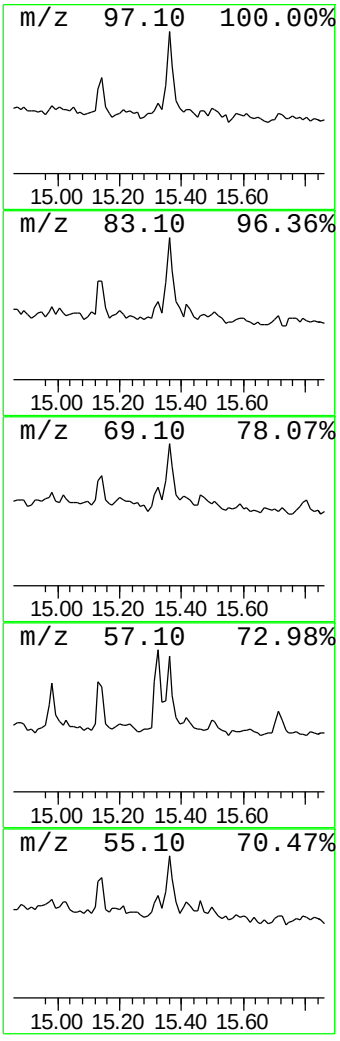
Peak Number 14 1-Heptacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	5.12 ng	165014	Perylene-d12	14.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
3	1-Heneicosanol	312	C21H44O	015594-90-8	86
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	83
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092916\
Data File : BF090296.D
Acq On : 29 Sep 2016 18:22
Operator : UM/SJ
Sample : H4982-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-25

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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...	4.55	20.0	ng	753885	1	6.46	752325	20.0
unknown6.23	6.23	93.0	ng	3496870	1	6.46	752325	20.0
Heptadecane	10.43	3.8	ng	189605	4	10.97	1008480	20.0
1-Pentadecene	11.23	3.3	ng	163633	4	10.97	1008480	20.0
n-Hexadecanoic acid	11.54	5.8	ng	290570	4	10.97	1008480	20.0
4H-Cyclopenta[def...	11.58	2.3	ng	114501	4	10.97	1008480	20.0
Octadecanoic acid	12.32	2.2	ng	136654	5	13.59	1225610	20.0
Behenic alcohol	13.47	7.7	ng	474121	5	13.59	1225610	20.0
Squalene	14.46	8.3	ng	265848	6	14.91	644824	20.0
Oxirane, hexadecyl-	15.14	3.4	ng	110114	6	14.91	644824	20.0
1-Heptacosanol	15.36	5.1	ng	165014	6	14.91	644824	20.0