LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

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-BF042716.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	4.967	250	252	259	rBV	18093	29104	2.59%	0.196%
2	5.390	286	289	291	rBV	770643	989921	88.02%	6.657%
3	5.619	306	309	315	rVB	7687	16429	1.46%	0.110%
4	5.847	326	329	336	rVB2	5970	19345	1.72%	0.130%
5	6.430	378	380	382	rBV	1118781	1060093	94.26%	7.129%
6	6.567	389	392	394	rBV	1177499	1124592	100.00%	7.563%
7	6.636	396	398	400	rVV2	20821	34438	3.06%	0.232%
8	6.682	400	402	405	rVB	9882	13914	1.24%	0.094%
9	6.807	410	413	415	rBV	508908	719124	63.95%	4.836%
10	6.956	424	426	429	rBV	968637	856081	76.12%	5.757%
11	7.070	434	436	438	rVB2	8729	15144	1.35%	0.102%
12	7.367	459	462	464	rBV	526772	594056	52.82%	3.995%
13	7.664	486	488	491	rVB	24448	24825	2.21%	0.167%
14	8.087	523	525	534	rBV	1126080	1062731	94.50%	7.147%
15	8.305	542	544	548	rVB3	11413	13416	1.19%	0.090%
16	8.362	548	549	554	rBV	17282	24589	2.19%	0.165%
17	8.796	584	587	592	rVB	7330	11621	1.03%	0.078%
18	9.162	617	619	622	rBV	1183062	1109952	98.70%	7.464%
19	9.253	625	627	629	rVV	18240	30851	2.74%	0.207%
20	9.287	629	630	635	rVB4	20082	33605	2.99%	0.226%
21	9.562	652	654	658	rBV	84274	92712	8.24%	0.623%
22	9.699	665	666	669	rBV2	7815	11775	1.05%	0.079%
23	9.779	672	673	676	rBV	29302	29078	2.59%	0.196%
24	9.836	676	678	681	rBV	889864	938758	83.48%	6.313%
25	10.019	690	694	695	rBV4	6696	15009	1.33%	0.101%
26	10.282	712	717	718	rBV	36615	46829	4.16%	0.315%
27	10.499	733	736	739	rBV	23154	30125	2.68%	0.203%
28	10.625	745	747	756	rBV	450740	523163	46.52%	3.518%
29	10.751	756	758	762	rVB	62065	81478	7.25%	0.548%
30	10.956	772	776	777	rBV3	10427	20165	1.79%	0.136%
31	11.196	796	797	798	rBV	34663	29431	2.62%	0.198%
32	11.231	798	800	803	rVB2	21407	25697	2.29%	0.173%
33	11.322	806	808	810	rBV	713717	773844	68.81%	5.204%
34	11.573	826	830	833	rBV5	14274	41918	3.73%	0.282%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

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-BF042716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.619	833	834	836	rVB	12898	13755	1.22%	0.093%
36	11.722	841	843	846	rBV3	7328	13429	1.19%	0.090%
37	11.791	846	849	850	rBV2	5891	12213	1.09%	0.082%
38	11.825	850	852	853	rBV	15211	17345	1.54%	0.117%
39	11.928	859	861	862	rBV	24608	26466	2.35%	0.178%
40	12.031	866	870	871	rBV	28460	34129	3.03%	0.230%
41	12.134	875	879	882	rVB4	9885	33449	2.97%	0.225%
42	12.248	887	889	892	rBV3	9868	15614	1.39%	0.105%
43	12.316	892	895	897	rBV3	11304	24746	2.20%	0.166%
44	12.374	897	900	901	rBV	25850	31448	2.80%	0.211%
45	12.419	903	904	906	rVB	24015	24436	2.17%	0.164%
46	12.534	912	914	916	rBV	83098	121097	10.77%	0.814%
47	12.739	930	932	935	rBV2	224531	361845	32.18%	2.433%
48	12.899	944	946	950	rBV	524530	755790	67.21%	5.083%
49	13.151	966	968	969	rBV2	44337	53764	4.78%	0.362%
50	13.185	969	971	976	rVV4	22813	60226	5.36%	0.405%
51	13.345	983	985	987	rBV2	41688	45826	4.07%	0.308%
52	13.436	991	993	995	rBV2	133760	164420	14.62%	1.106%
53	13.482	995	997	999	rBV	49982	89813	7.99%	0.604%
54	13.814	1024	1026	1030	rBV2	74448	111112	9.88%	0.747%
55	13.951	1035	1038	1044	rBV	665519	1009390	89.76%	6.788%
56	14.134	1052	1054	1055	rBV	83037	78534	6.98%	0.528%
57	15.048	1132	1134	1137	rVB	126591	161005	14.32%	1.083%
58	15.368	1159	1162	1164	rBV	440076	613546	54.56%	4.126%
59	15.814	1199	1201	1203	rBV	108944	180996	16.09%	1.217%
60	16.020	1217	1219	1228	rVB2	157161	371976	33.08%	2.501%

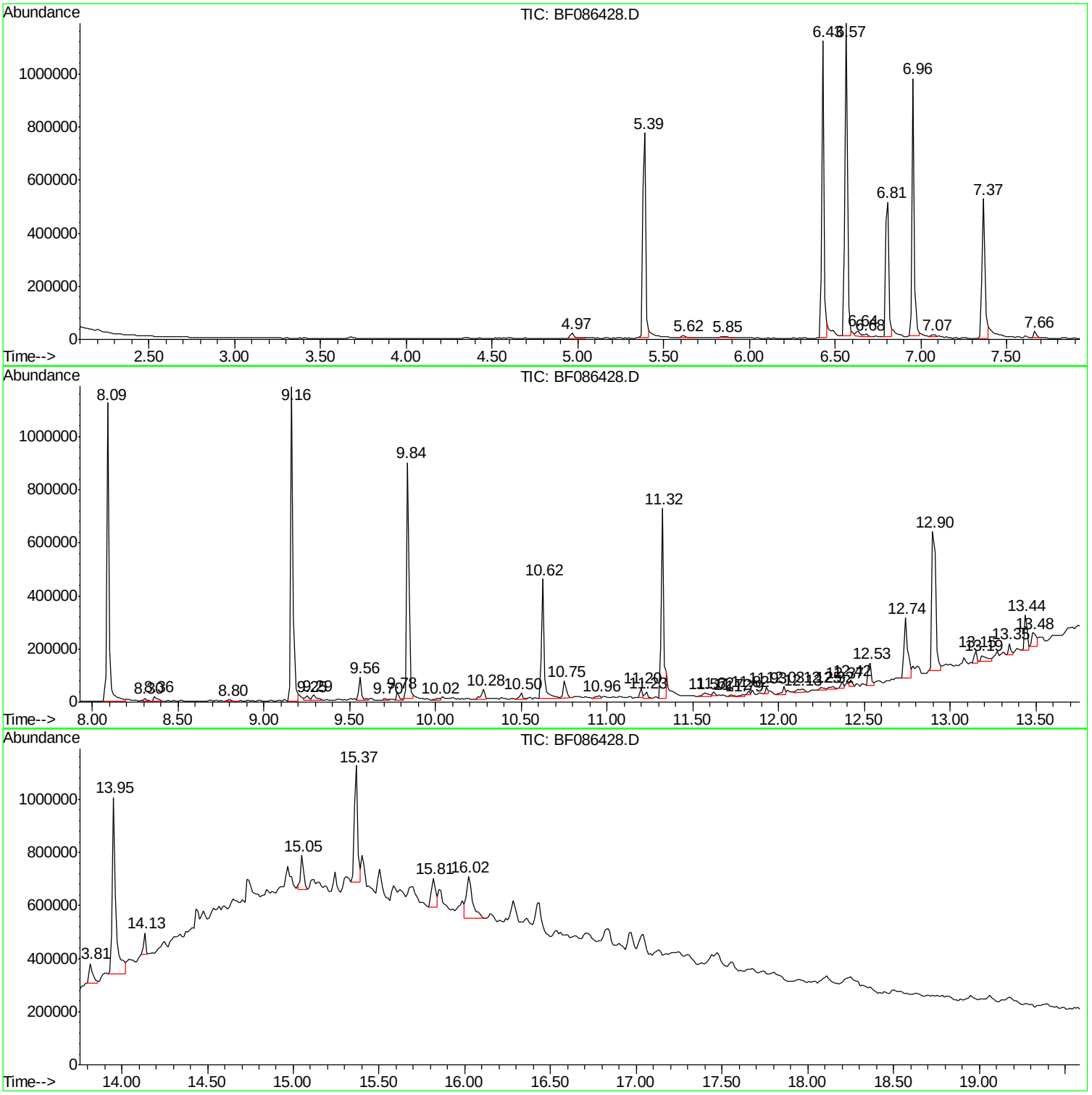
Sum of corrected areas: 14870183

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WPG-B5(0-5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

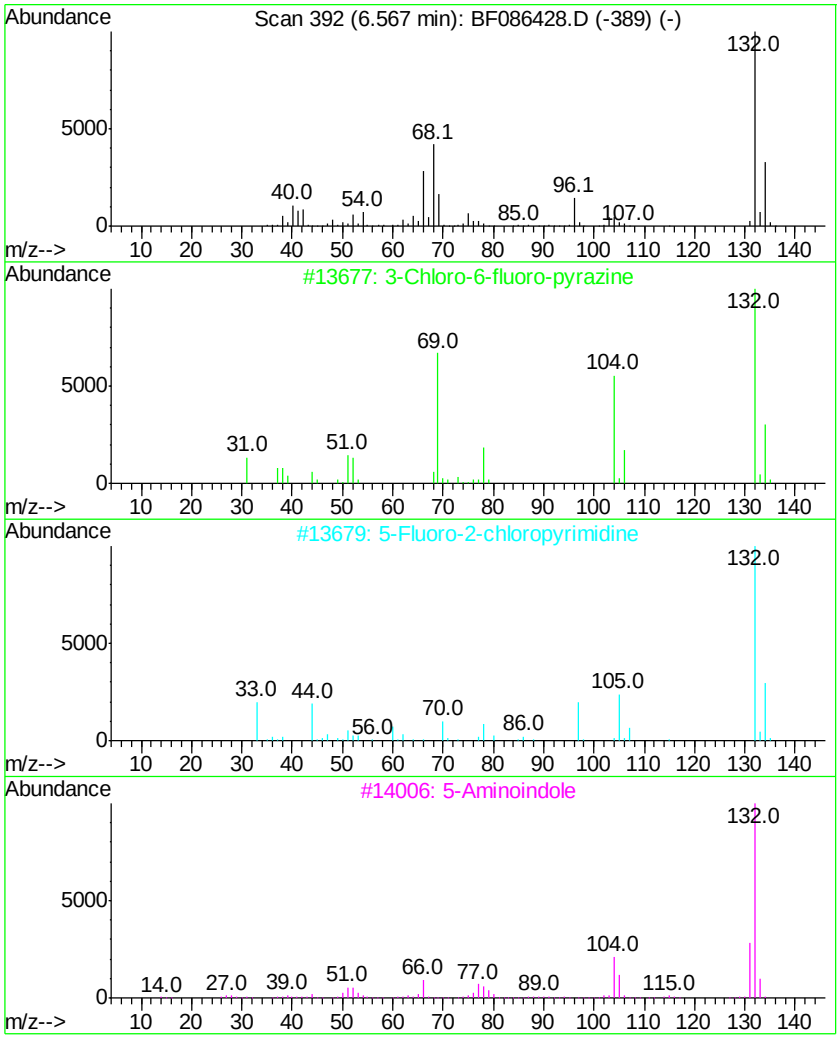
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

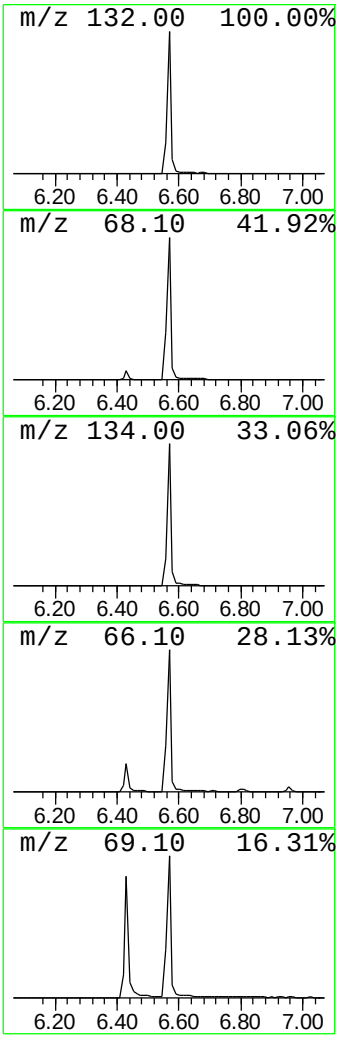
****

Peak Number 1 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	31.28 ng	1124590	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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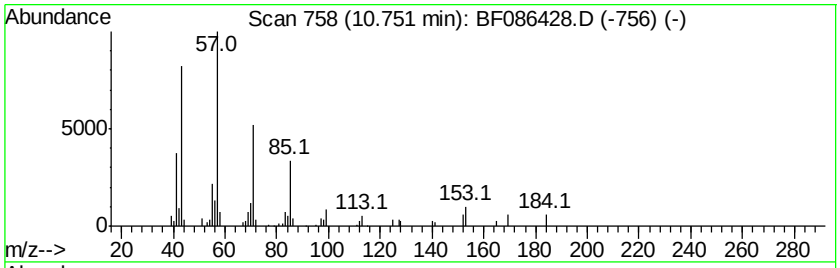
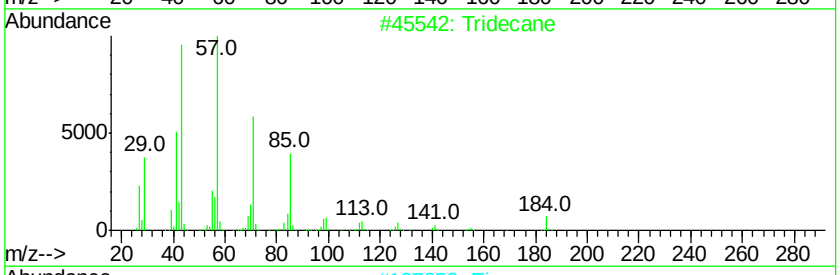
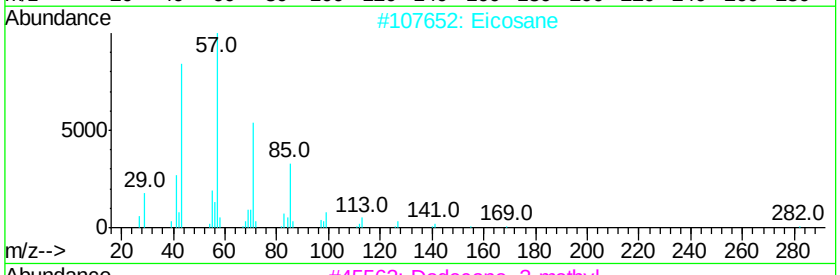
Peak Number 3 Tridecane Concentration Rank 8

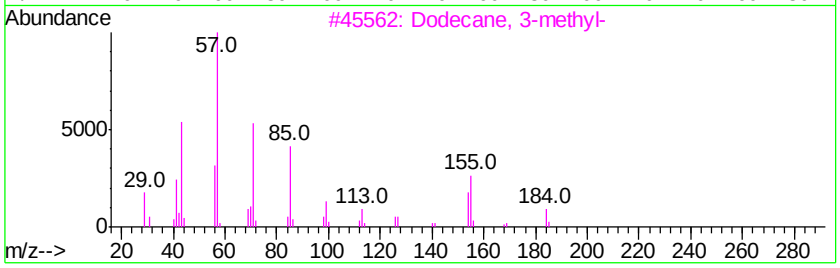
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.11 ng	81478	Phenanthrene-d10	11.32

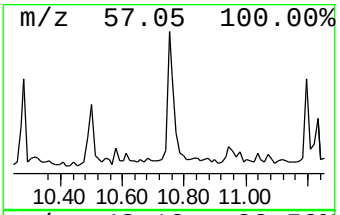
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Eicosane	282	C20H42	000112-95-8	81
3	Dodecane, 3-methyl-	184	C13H28	017312-57-1	72
4	Hexadecane	226	C16H34	000544-76-3	72
5	Octadecane	254	C18H38	000593-45-3	72

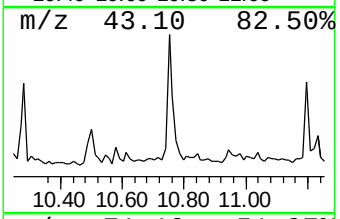


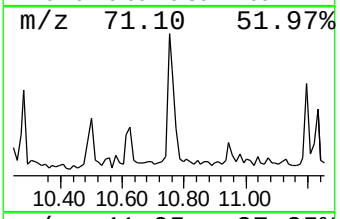


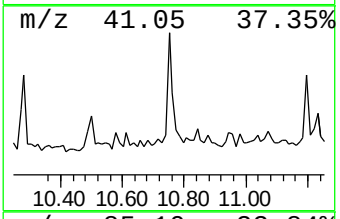


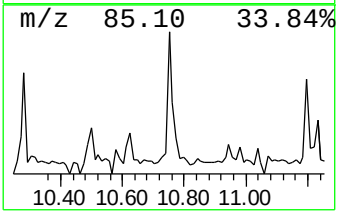












Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

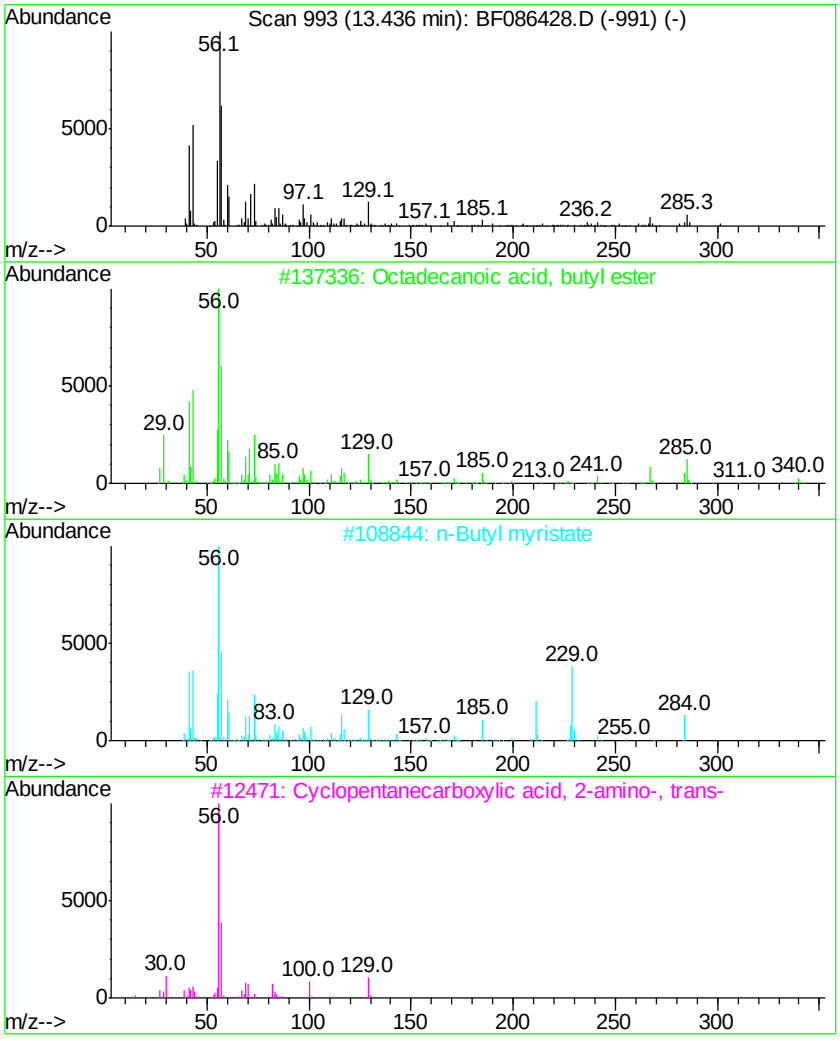
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

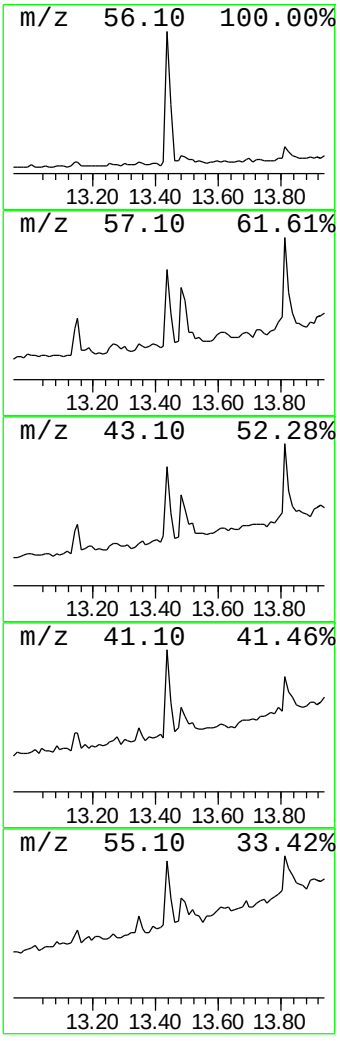
****

Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	3.26 ng	164420	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	n-Butyl myristate	284	C18H36O2	000110-36-1	78
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	46
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	43
5	Undecane, 5-methylene-	168	C12H24	005698-48-6	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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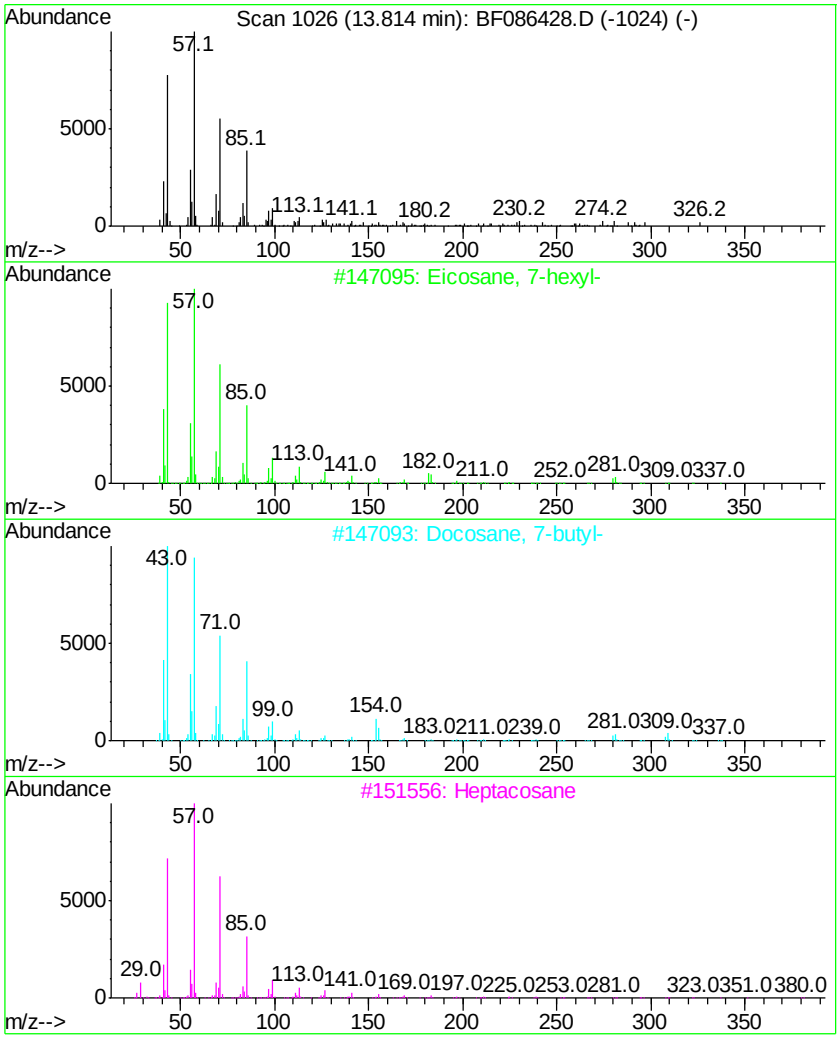
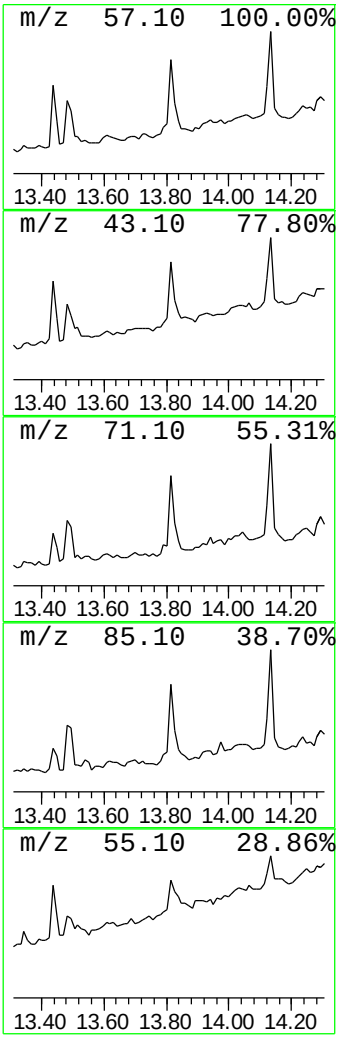
Peak Number 5 Eicosane, 7-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	2.20 ng	111112	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
2	Docosane, 7-butyl-	366	C26H54	055282-15-0	86
3	Heptacosane	380	C27H56	000593-49-7	83
4	Eicosane	282	C20H42	000112-95-8	83
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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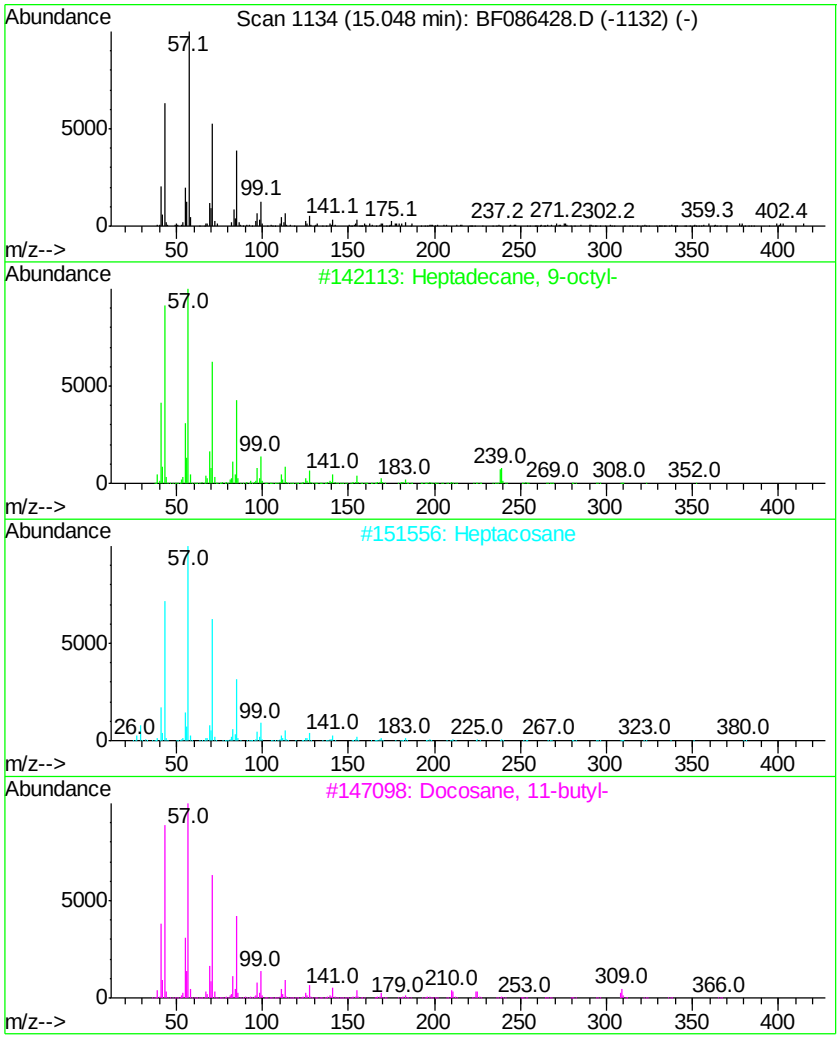
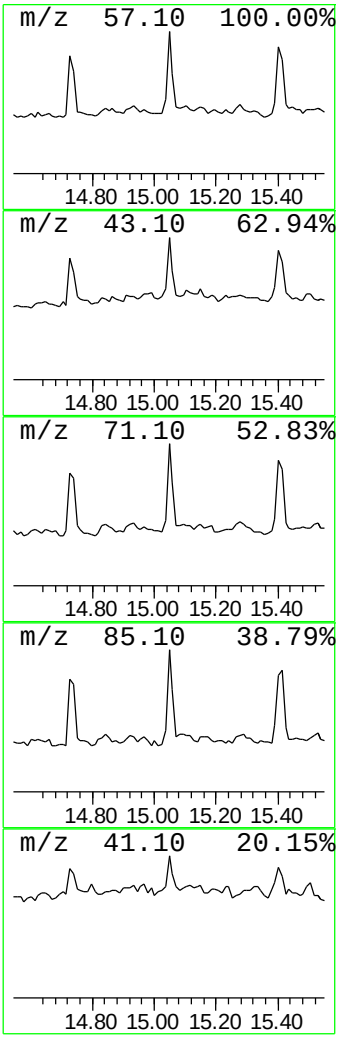
Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	5.25 ng	161005	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	98
2	Heptacosane	380	C27H56	000593-49-7	98
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	98
4	Octacosane	394	C28H58	000630-02-4	94
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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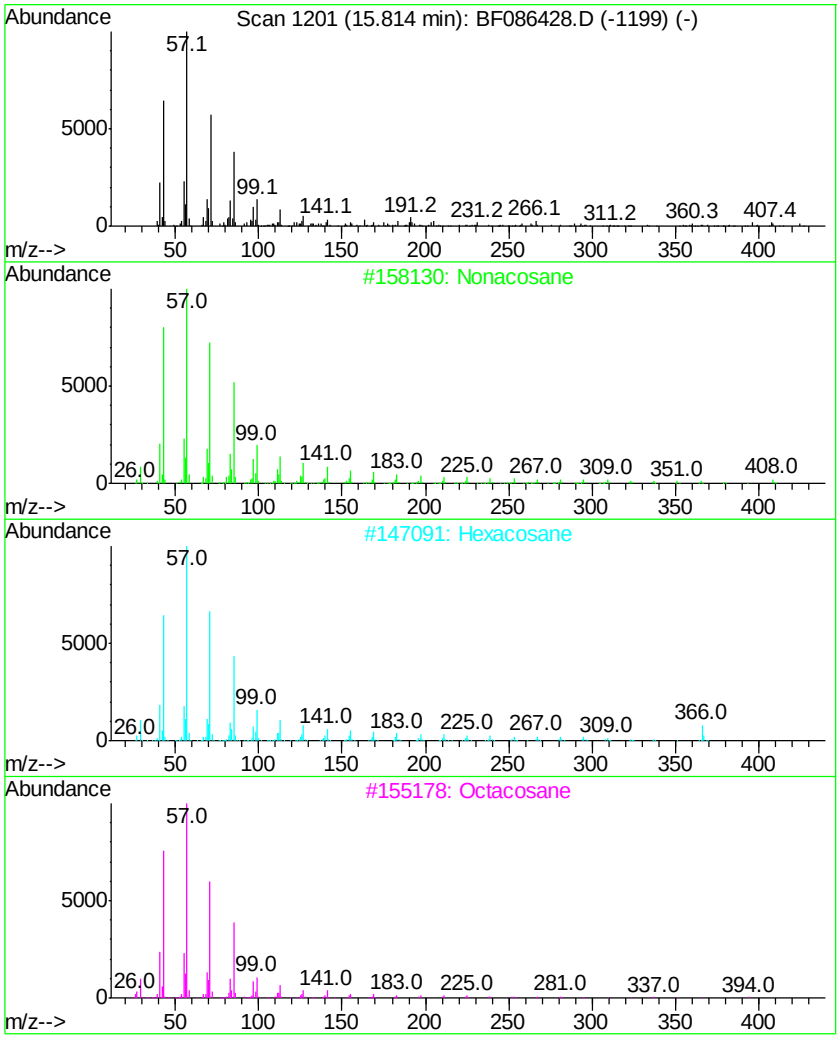
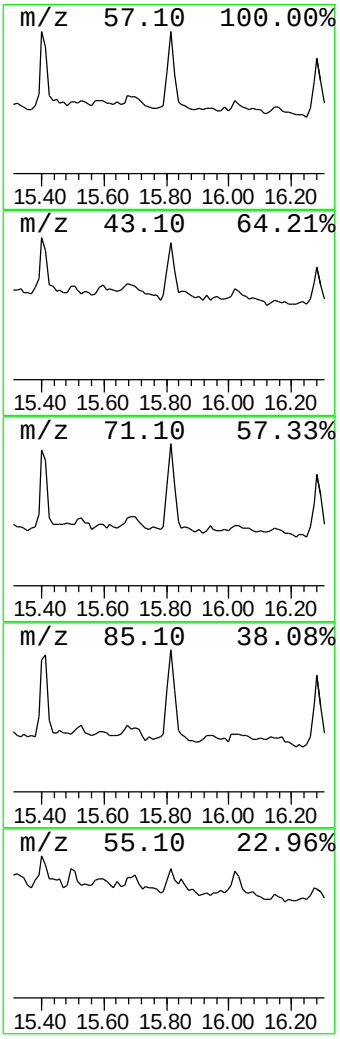
Peak Number 7 Nonacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	5.90 ng	180996	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosane	408	C29H60	000630-03-5	93
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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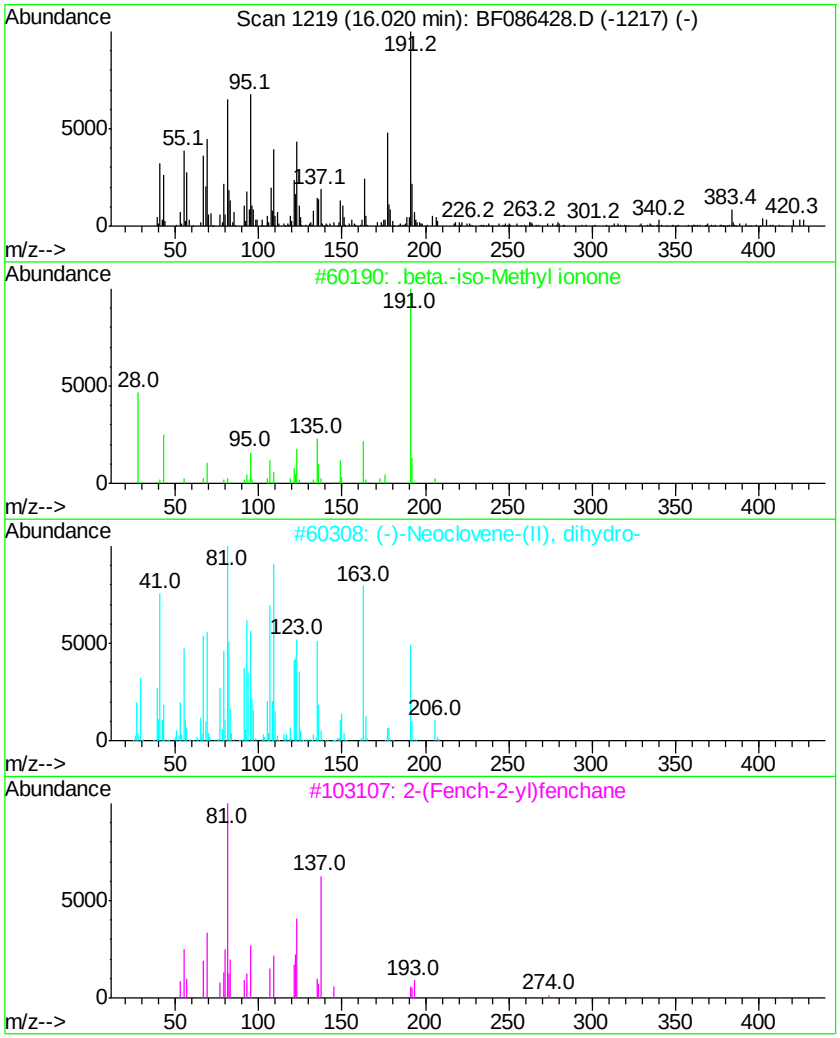
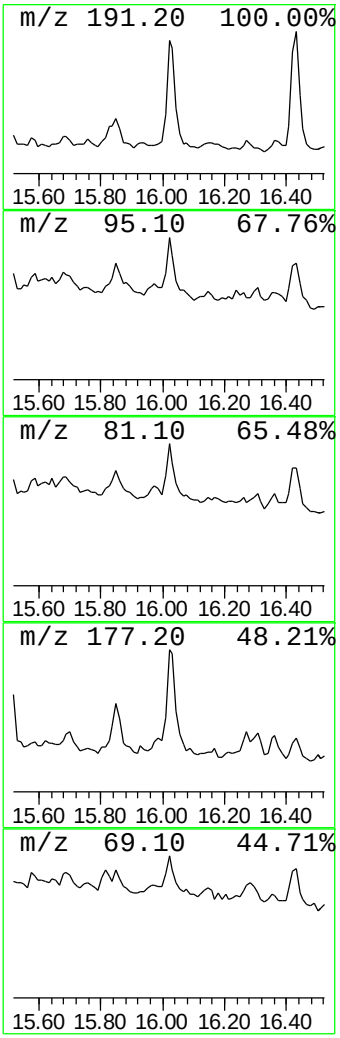
Peak Number 8 .beta.-iso-Methyl ionone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	12.13 ng	371976	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	60
2	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	56
3	2-(Fench-2-yl)fenchane	274	C20H34	1000105-83-1	27
4	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	27
5	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042716\
Data File : BF086428.D
Acq On : 27 Apr 2016 17:10
Operator : UM/SJ
Sample : H2652-15 4X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPG-B5(0-5)-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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
unknown6.57	6.57	31.3	ng	1124590	1	6.81	719124	20.0
Tridecane	10.75	2.1	ng	81478	4	11.32	773844	20.0
Octadecanoic acid...	13.44	3.3	ng	164420	5	13.95	1009390	20.0
Eicosane, 7-hexyl-	13.81	2.2	ng	111112	5	13.95	1009390	20.0
Heptadecane, 9-oc...	15.05	5.3	ng	161005	6	15.37	613546	20.0
Nonacosane	15.81	5.9	ng	180996	6	15.37	613546	20.0
.beta.-iso-Methyl...	16.02	12.1	ng	371976	6	15.37	613546	20.0