LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)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-BF060716.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	1.667	6	7	12	rVV	22748	33157	1.86%	0.182%
2	1.781	15	17	24	rVV	211732	277545	15.56%	1.524%
3	1.873	24	25	31	rVB	37228	59550	3.34%	0.327%
4	4.844	283	285	290	rBV	70768	96800	5.43%	0.531%
5	4.913	290	291	294	rVB	17243	19073	1.07%	0.105%
6	5.290	321	324	326	rBV	1597038	1784028	100.00%	9.794%
7	5.679	355	358	360	rVB2	14992	23945	1.34%	0.131%
8	5.816	368	370	372	rVB	20457	21754	1.22%	0.119%
9	5.873	372	375	377	rBV2	14590	24829	1.39%	0.136%
10	5.919	377	379	382	rVB	57299	71339	4.00%	0.392%
11	5.976	382	384	386	rBV	34691	39567	2.22%	0.217%
12	6.113	393	396	402	rBV	27861	52742	2.96%	0.290%
13	6.205	402	404	406	rBV2	28621	43226	2.42%	0.237%
14	6.342	413	416	419	rBV2	1482145	1674643	93.87%	9.194%
15	6.422	421	423	424	rBV	30067	42891	2.40%	0.235%
16	6.456	424	426	429	rVV	1710576	1643146	92.10%	9.021%
17	6.536	431	433	435	rVB2	23805	34925	1.96%	0.192%
18	6.616	438	440	442	rBV2	16108	30767	1.72%	0.169%
19	6.685	444	446	450	rVB	605817	531109	29.77%	2.916%
20	6.753	450	452	453	rBV2	16762	28353	1.59%	0.156%
21	6.810	456	457	458	rVV	53991	50925	2.85%	0.280%
22	6.845	458	460	462	rVV	1471394	1543623	86.52%	8.474%
23	6.925	464	467	468	rVV3	23548	40164	2.25%	0.220%
24	6.959	468	470	473	rVV2	27349	46639	2.61%	0.256%
25	7.039	475	477	479	rVV3	17959	23819	1.34%	0.131%
26	7.073	479	480	482	rVV	30959	41545	2.33%	0.228%
27	7.107	482	483	487	rVV2	22227	41710	2.34%	0.229%
28	7.210	490	492	493	rVV2	27410	43624	2.45%	0.239%
29	7.256	493	496	498	rVV	1093263	1095705	61.42%	6.015%
30	7.336	501	503	506	rVV3	32555	70914	3.97%	0.389%
31	7.382	506	507	512	rVV	32287	43590	2.44%	0.239%
32	7.496	515	517	519	rVB	45700	44371	2.49%	0.244%
33	7.610	523	527	530	rVB3	32114	61782	3.46%	0.339%
34	7.736	535	538	541	rVB2	18661	35124	1.97%	0.193%

LSC Area Percent Report

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Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	7.885	545	551	553	rBV5	14303	50918	2.85%	0.280%
36	7.976	556	559	561	rBV	577663	637404	35.73%	3.499%
37	8.262	581	584	586	rBV2	21287	37661	2.11%	0.207%
38	8.410	594	597	601	rVB	79471	136329	7.64%	0.748%
39	8.662	618	619	622	rVB	20489	28477	1.60%	0.156%
40	8.788	625	630	633	rVB7	14111	43636	2.45%	0.240%
41	8.856	633	636	637	rBV3	25264	33414	1.87%	0.183%
42	8.890	637	639	641	rVB2	17041	24796	1.39%	0.136%
43	9.005	647	649	650	rVB	89903	71574	4.01%	0.393%
44	9.050	650	653	655	rBV	1823131	1606277	90.04%	8.818%
45	9.153	658	662	663	rBV4	20743	52680	2.95%	0.289%
46	9.176	663	664	669	rVB4	15789	38481	2.16%	0.211%
47	9.302	672	675	676	rBV2	10441	19979	1.12%	0.110%
48	9.382	681	682	684	rBV	19347	25699	1.44%	0.141%
49	9.451	684	688	690	rBV	627496	603351	33.82%	3.312%
50	9.633	702	704	705	rVB	29979	24020	1.35%	0.132%
51	9.668	705	707	708	rBV	41568	37610	2.11%	0.206%
52	9.725	708	712	714	rVV	638649	632229	35.44%	3.471%
53	9.839	720	722	723	rVB2	16517	20717	1.16%	0.114%
54	9.896	723	727	728	rBV	17600	33064	1.85%	0.182%
55	9.931	728	730	731	rVV	21384	33354	1.87%	0.183%
56	9.988	734	735	737	rVV	38778	28324	1.59%	0.155%
57	10.045	737	740	743	rVV4	9166	20877	1.17%	0.115%
58	10.159	749	750	754	rVB	52904	52077	2.92%	0.286%
59	10.376	766	769	772	rBV	58289	105033	5.89%	0.577%
60	10.514	778	781	783	rBV	708260	825459	46.27%	4.532%
61	10.594	786	788	790	rVB3	13177	20013	1.12%	0.110%
62	10.639	790	792	795	rBV	92085	174127	9.76%	0.956%
63	10.834	806	809	813	rVB4	13745	34449	1.93%	0.189%
64	11.085	829	831	832	rBV	25095	35517	1.99%	0.195%
65	11.108	832	833	836	rVB	46605	43416	2.43%	0.238%
66	11.199	839	841	845	rBV	614678	531227	29.78%	2.916%
67	11.268	845	847	850	rVB2	13708	21643	1.21%	0.119%
68	11.736	886	888	890	rBV3	13725	18626	1.04%	0.102%
69	11.805	892	894	899	rVB4	12198	31410	1.76%	0.172%
70	12.194	925	928	931	rBV5	10886	24544	1.38%	0.135%
71	12.411	945	947	948	rBV	27830	27716	1.55%	0.152%

LSC Area Percent Report

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Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	12.445	948	950	953	rVV4	14105	22972	1.29%	0.126%
73	12.639	965	967	968	rVB	20058	19050	1.07%	0.105%
74	12.788	977	980	982	rBV	806083	1108471	62.13%	6.085%
75	12.914	989	991	993	rVB	19411	18467	1.04%	0.101%
76	13.028	999	1001	1003	rBV2	15039	20603	1.15%	0.113%
77	13.702	1058	1060	1065	rVB	74076	122320	6.86%	0.672%
78	13.828	1069	1071	1074	rVV	544844	518432	29.06%	2.846%
79	13.931	1078	1080	1082	rVB	34320	38352	2.15%	0.211%
80	14.662	1142	1144	1146	rVB	38271	53087	2.98%	0.291%
81	15.211	1190	1192	1198	rVB	323866	390193	21.87%	2.142%

Sum of corrected areas: 18214999

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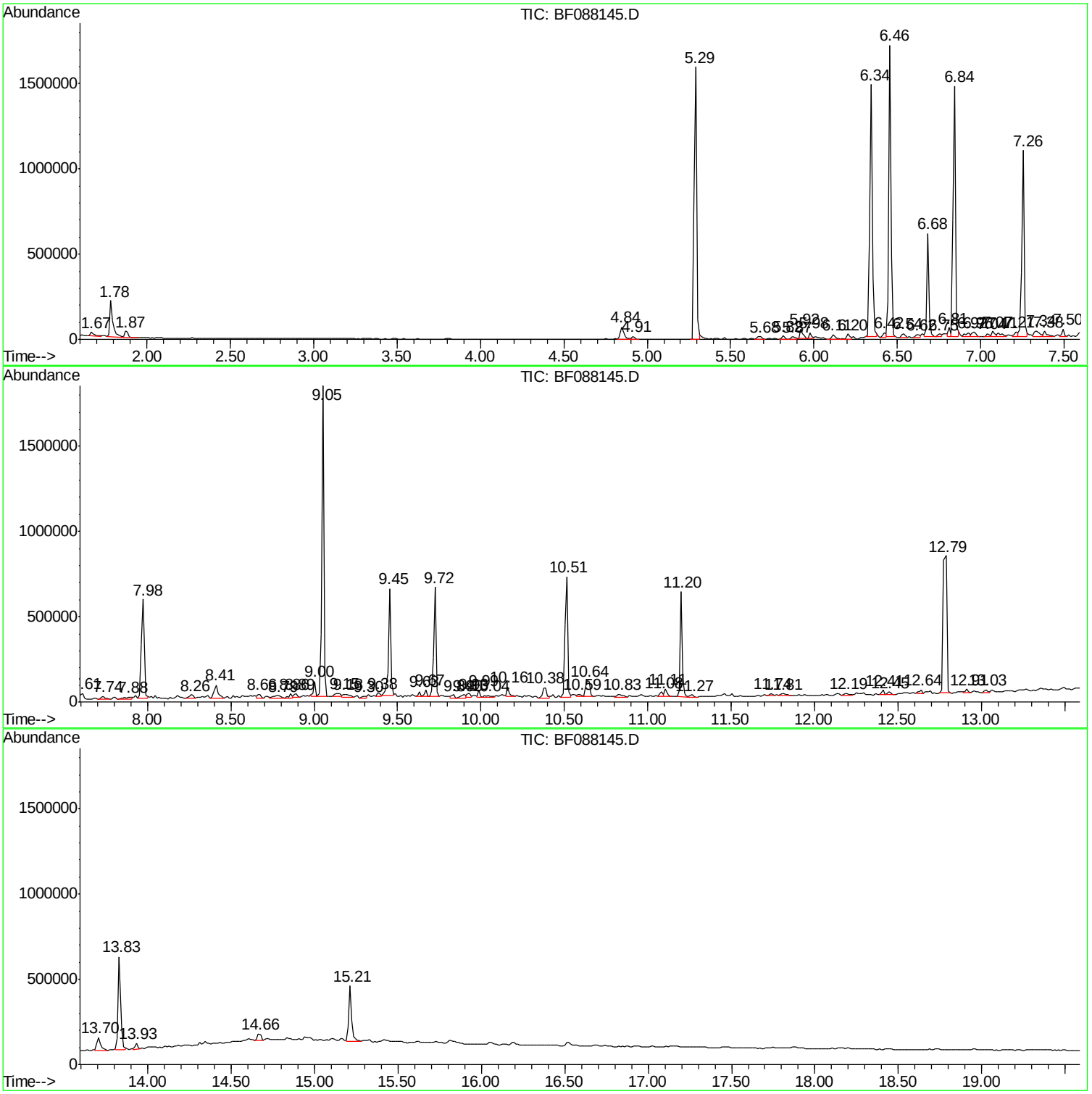
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF061816\
Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

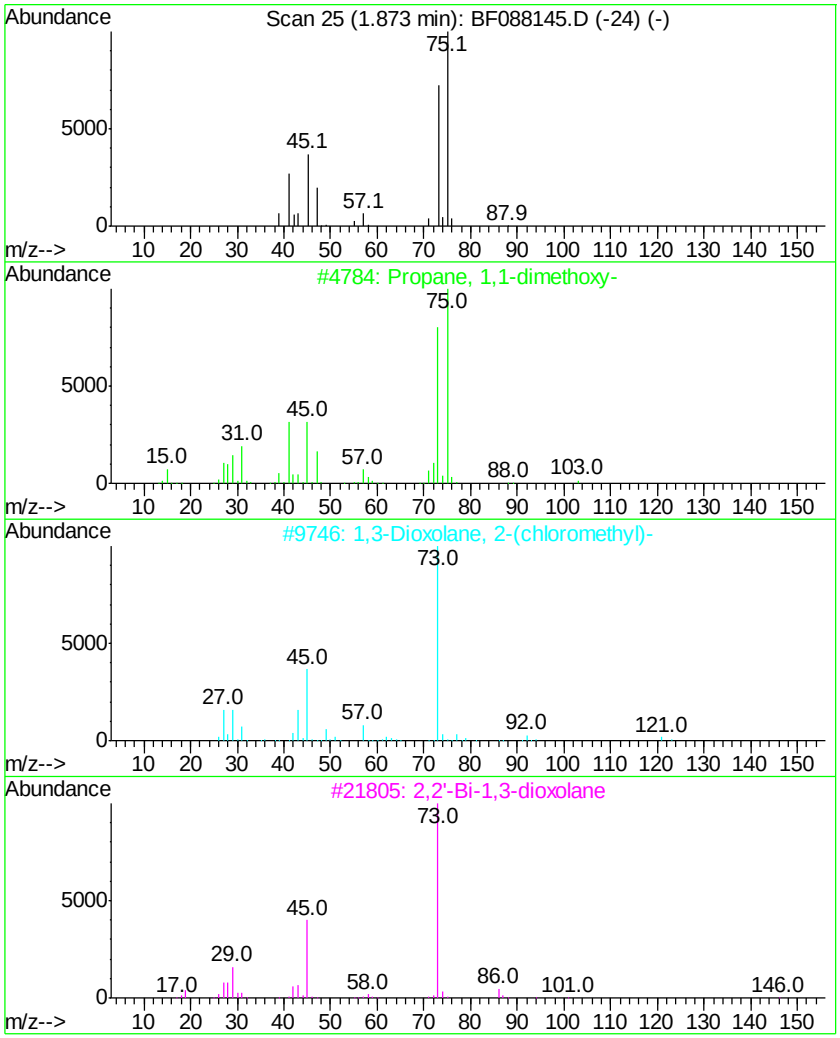
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

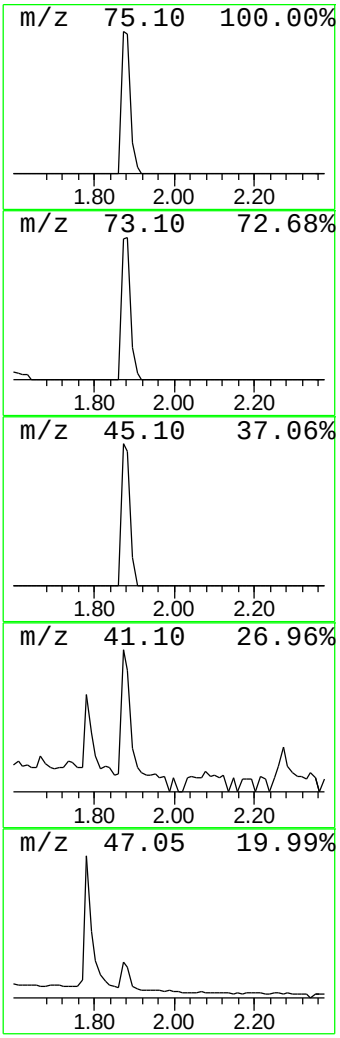
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.87	2.24 ng	59550	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
3	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
4	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
5	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	8





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

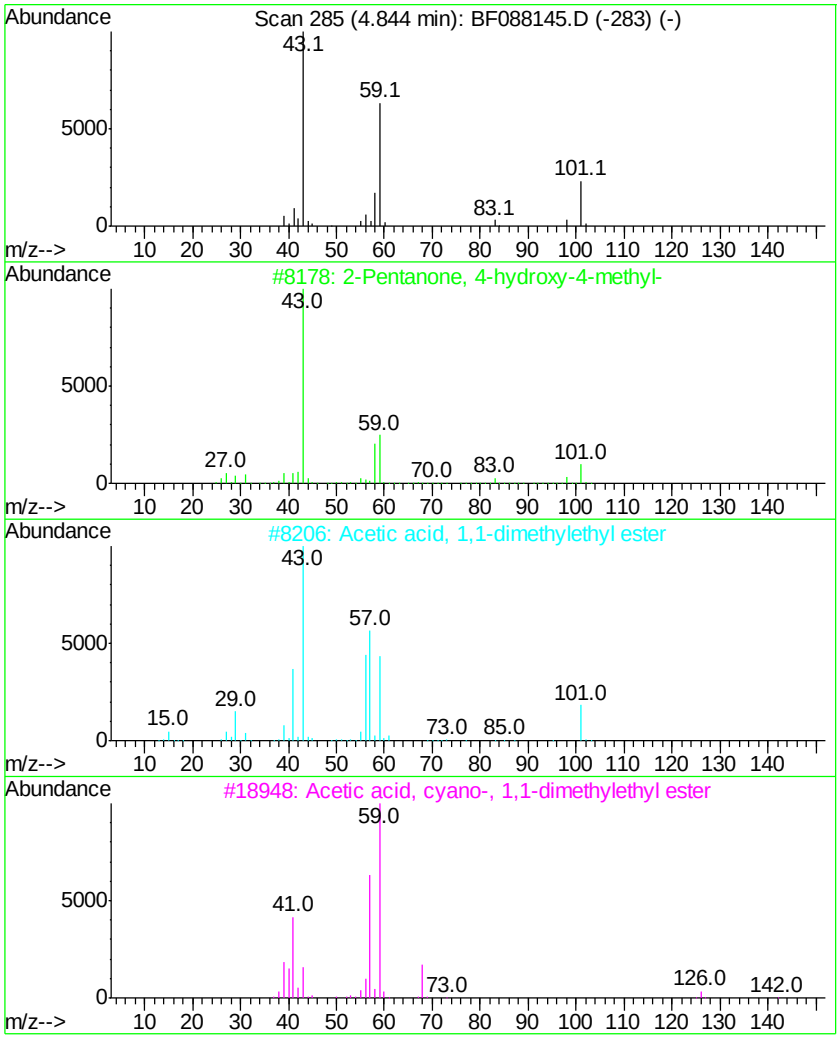
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

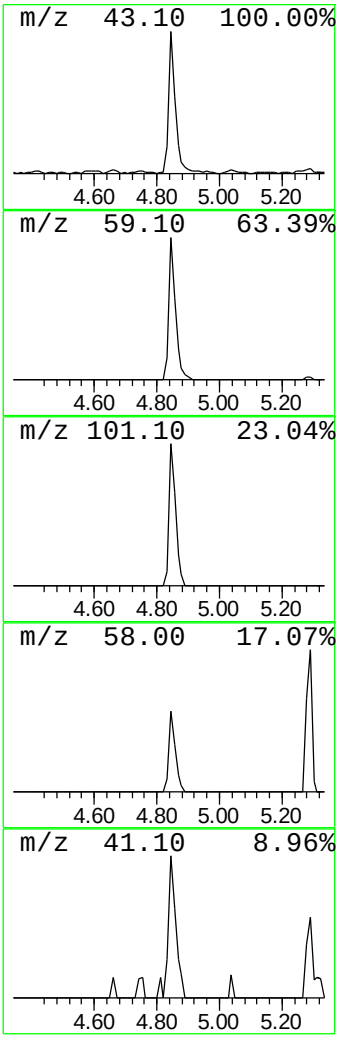
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	3.65 ng	96800	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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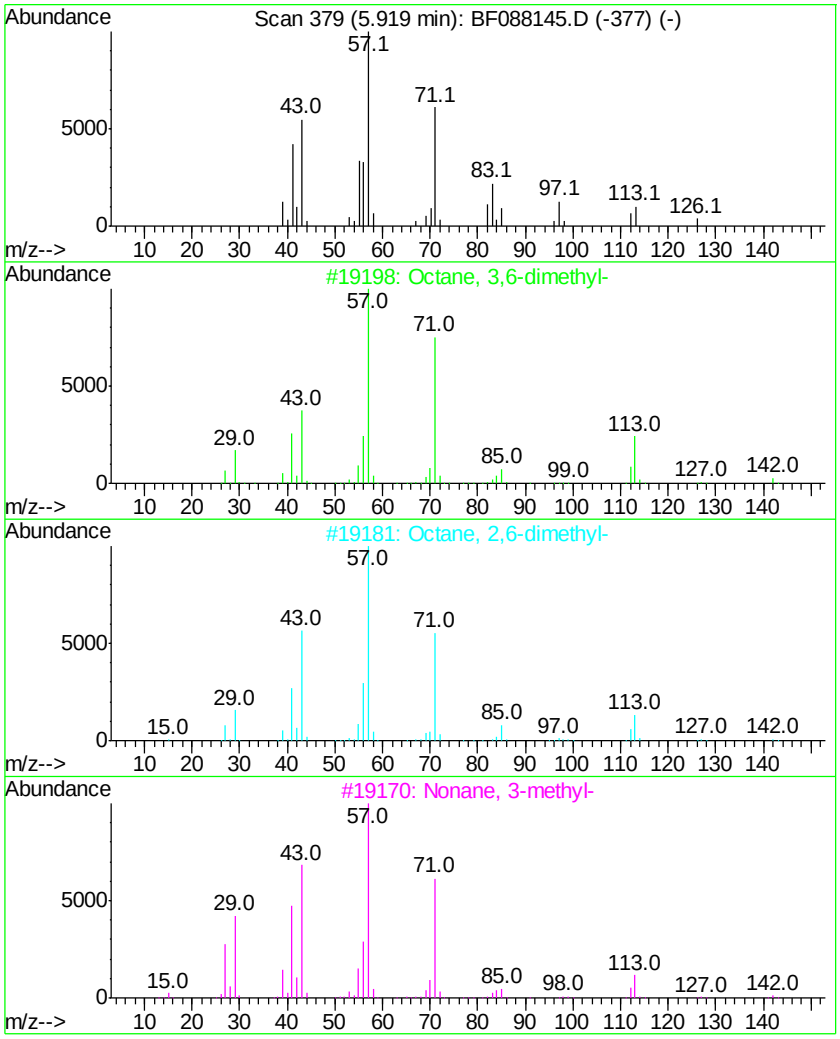
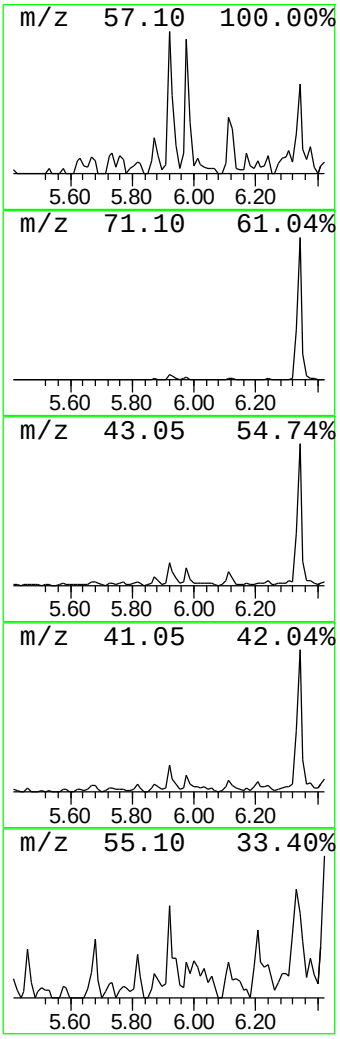
****

Peak Number 4 Octane, 3,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.92	2.69 ng	71339	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	58
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	47
5	Nonane, 4-methyl-5-propyl-	184	C13H28	062185-55-1	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

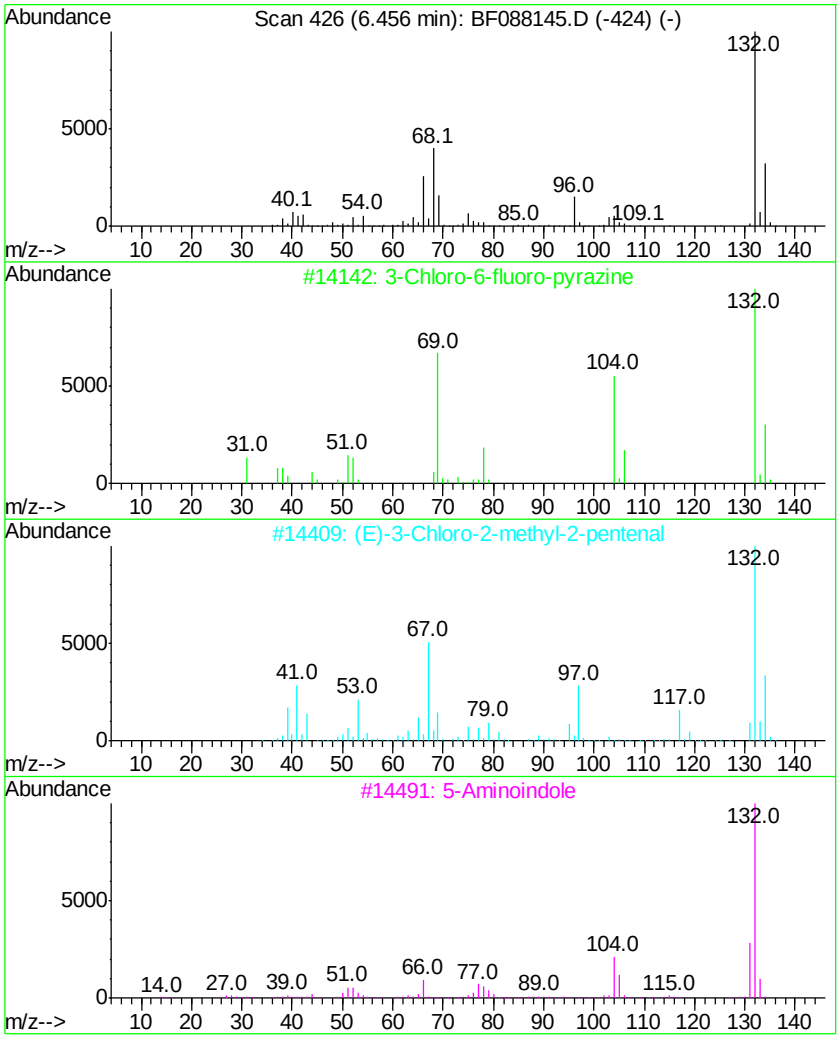
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

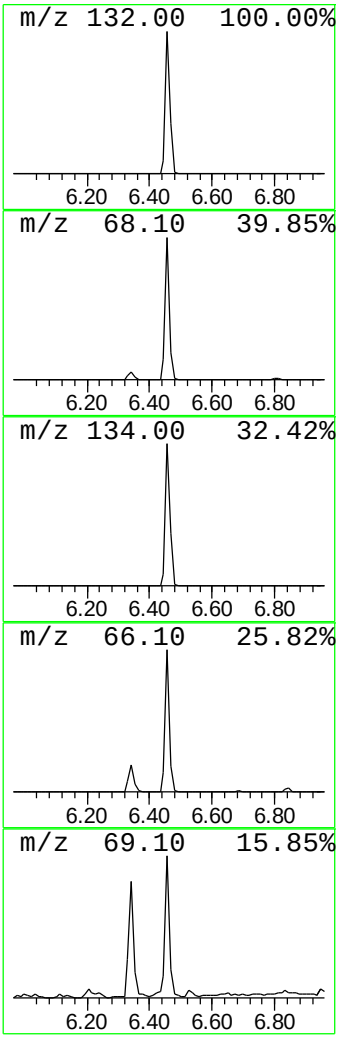
****

Peak Number 5 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	61.88 ng	1643150	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

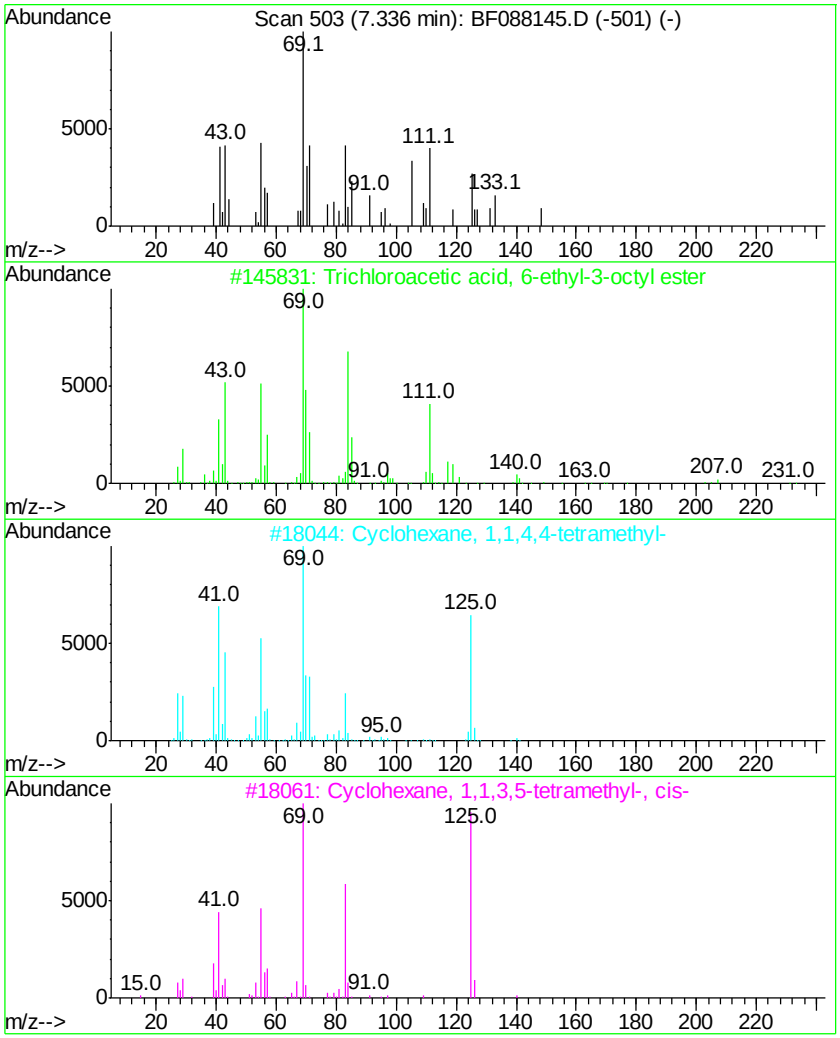
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

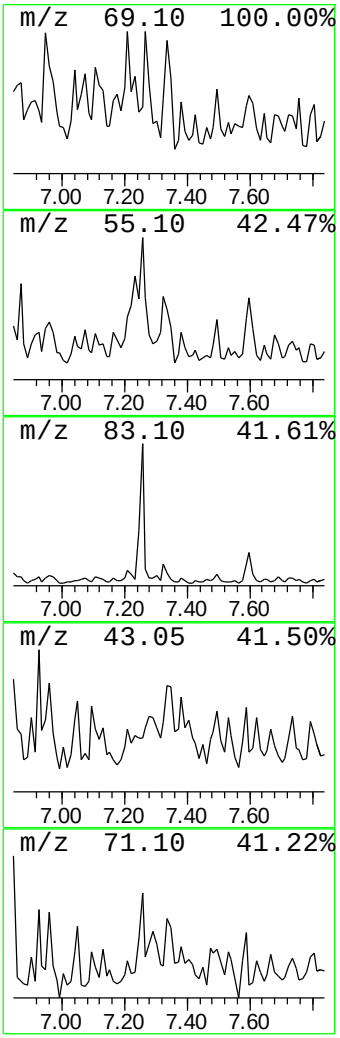
****

Peak Number 7 unknown7.34 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	2.23 ng	70914	Naphthalene-d8	7.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, 6-ethyl-3-...	302	C12H21Cl3O2	1000282-57-4	38
2	Cyclohexane, 1,1,4,4-tetramethyl-	140	C10H20	002223-52-1	38
3	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	38
4	Cyclohexane, 1-ethyl-2,3-dimethyl-	140	C10H20	007058-05-1	35
5	1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	35





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Data File : BF088145.D
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Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

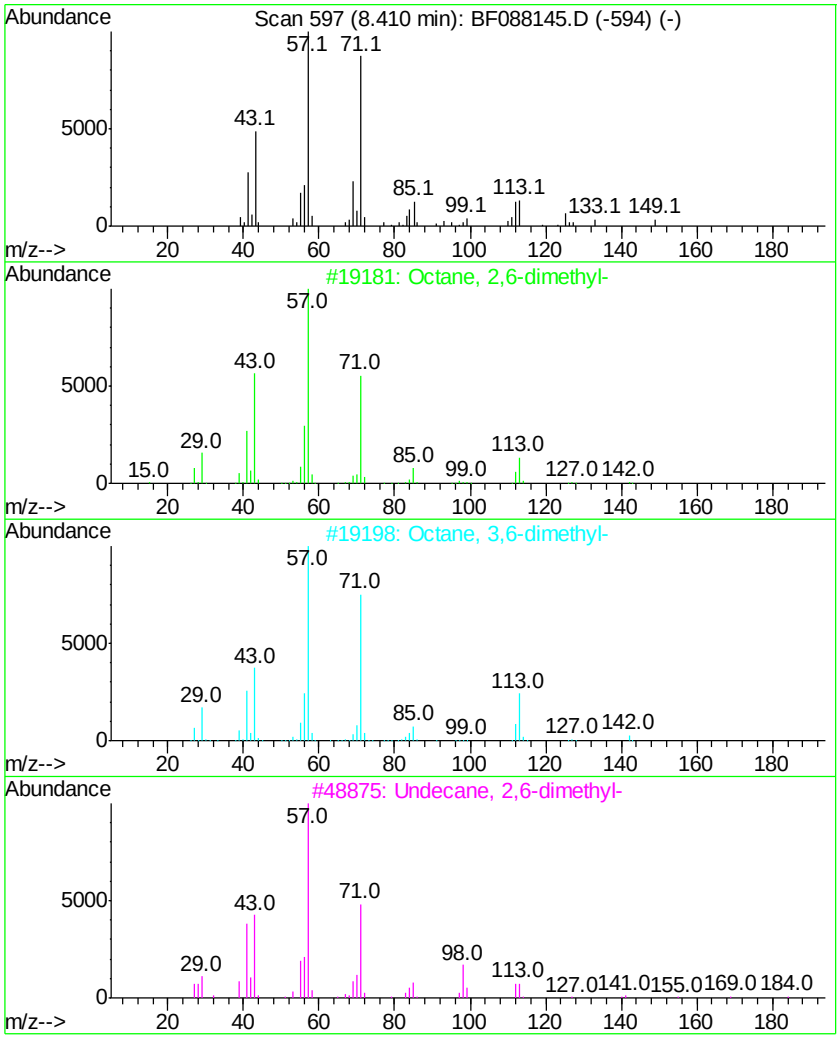
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

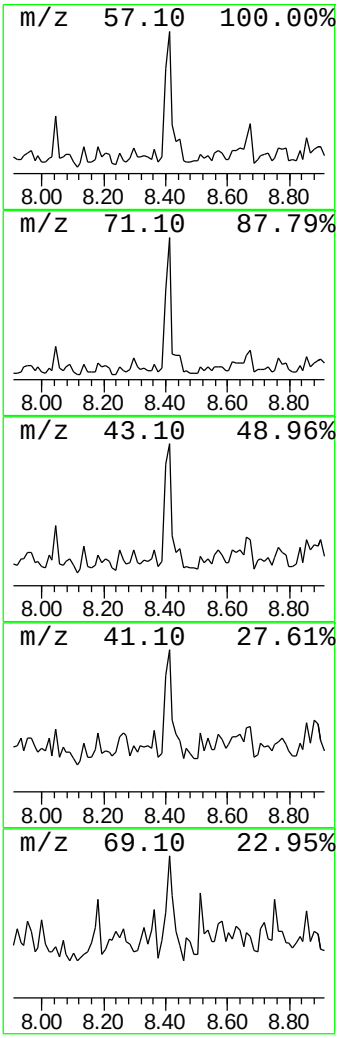
****

Peak Number 8 Octane, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	4.28 ng	136329	Naphthalene-d8	7.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	72
3	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	64
4	Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	59
5	Tridecane, 7-methyl-	198	C14H30	026730-14-3	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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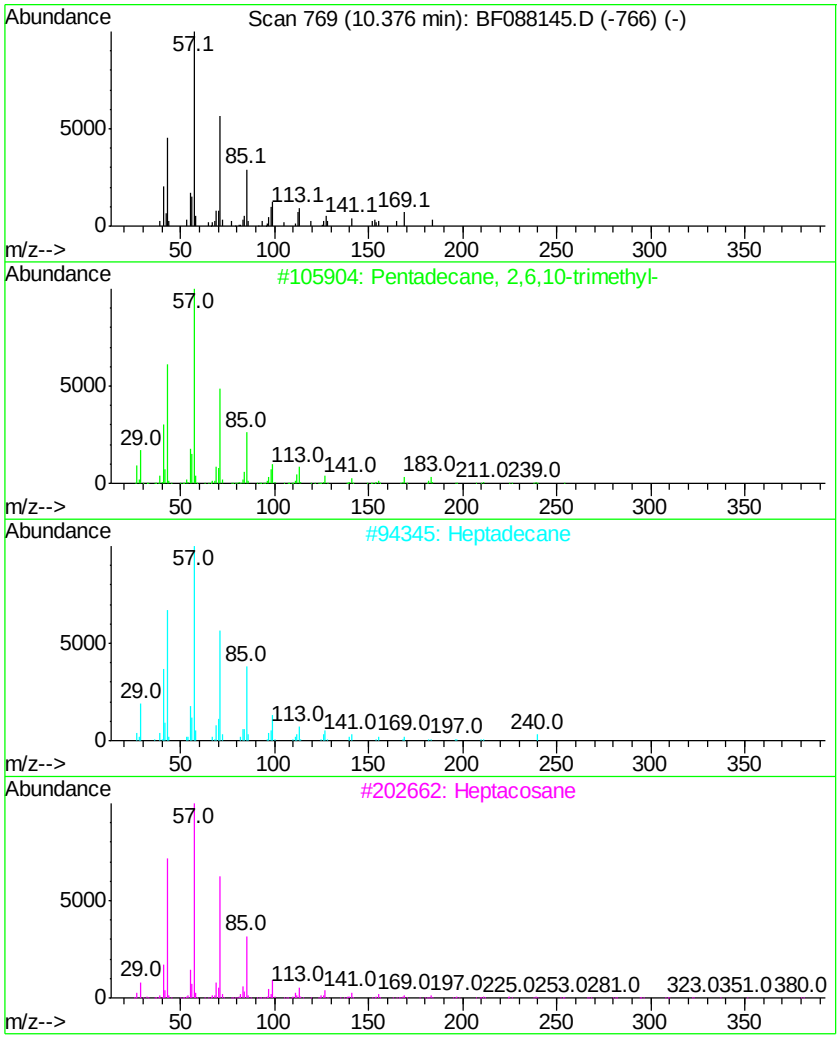
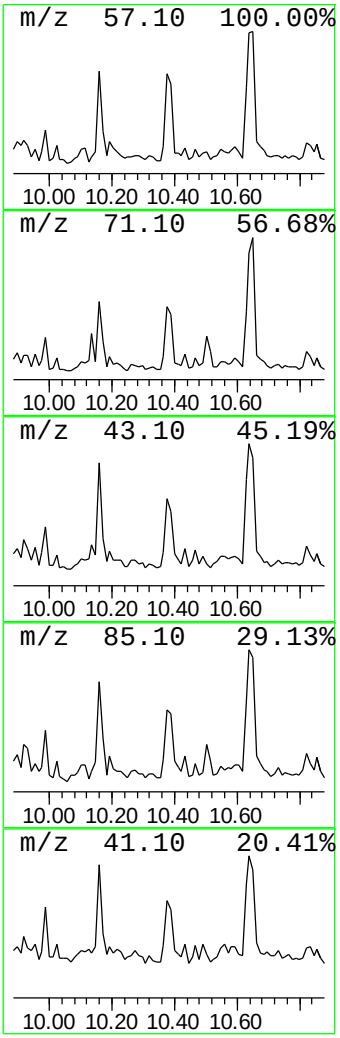
Peak Number 9 Pentadecane, 2,6,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	3.32 ng	105033	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
2	Heptadecane	240	C17H36	000629-78-7	86
3	Heptacosane	380	C27H56	000593-49-7	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Octadecane	254	C18H38	000593-45-3	78





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Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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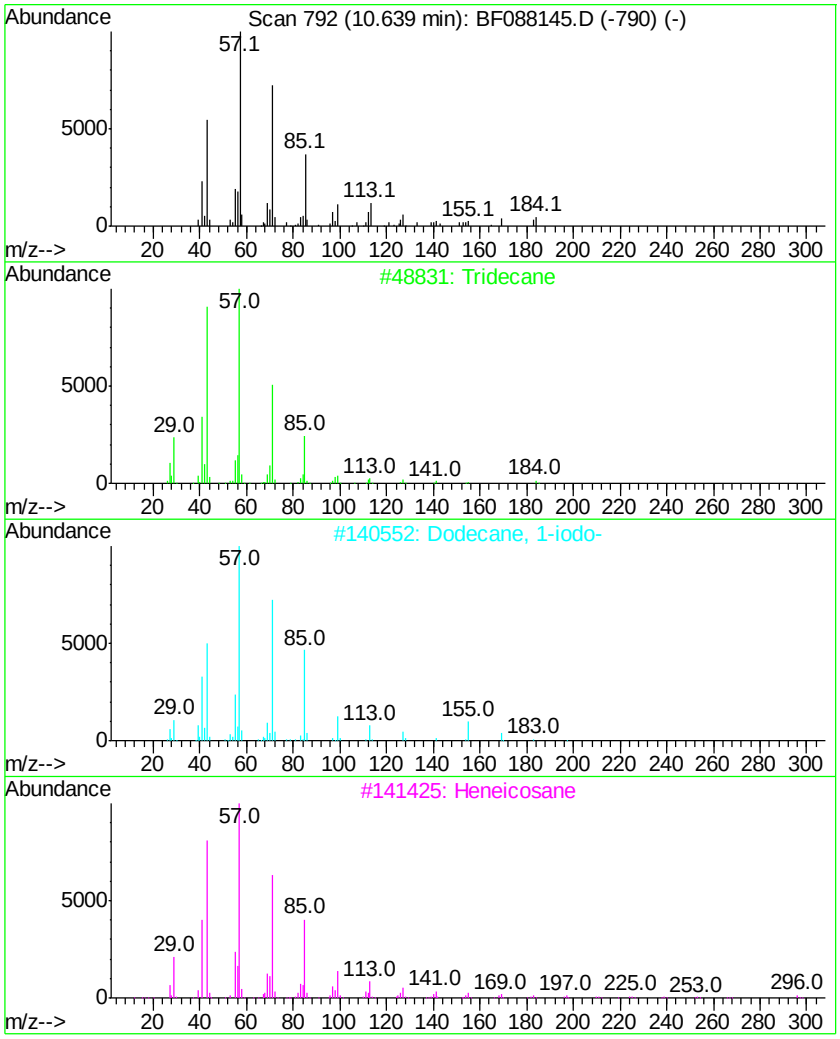
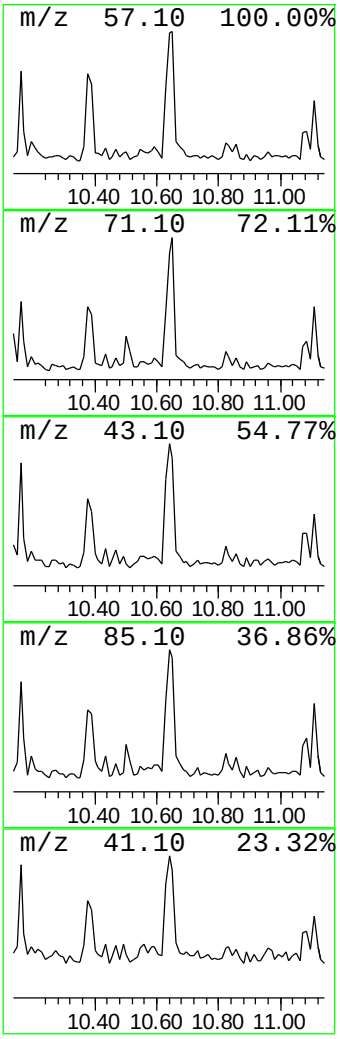
Peak Number 10 Tridecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	6.56 ng	174127	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	83
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
3	Heneicosane	296	C21H44	000629-94-7	80
4	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
5	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	72





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Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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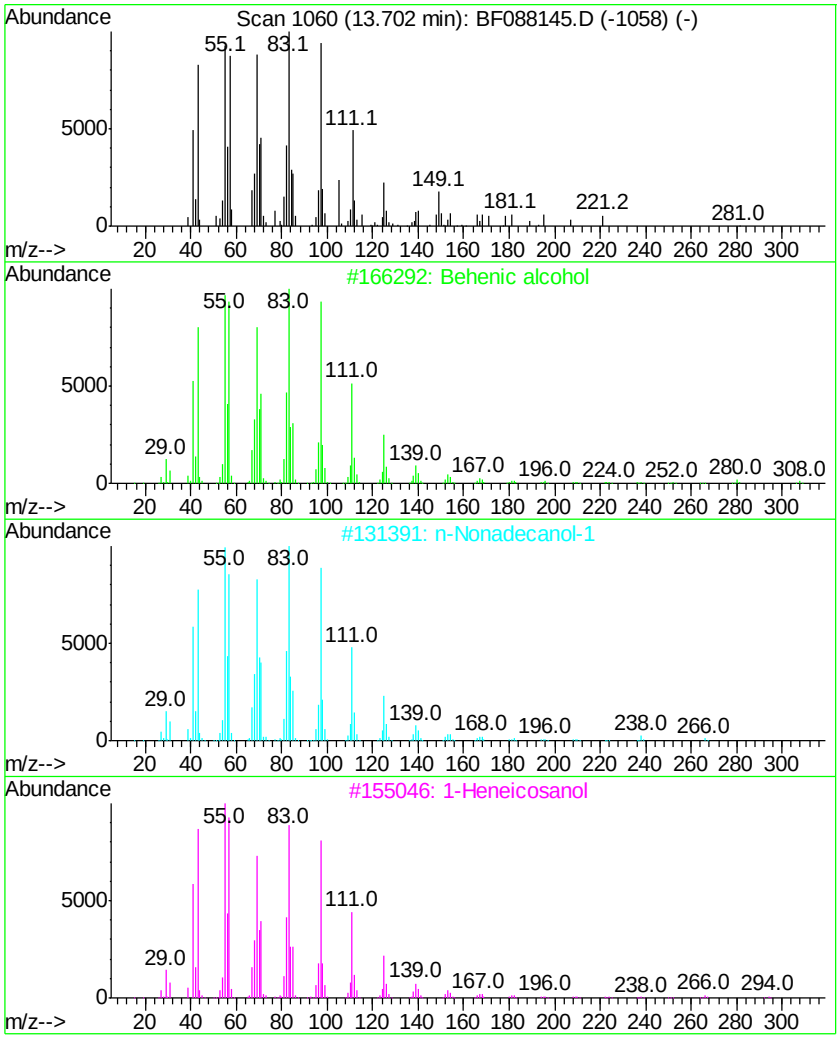
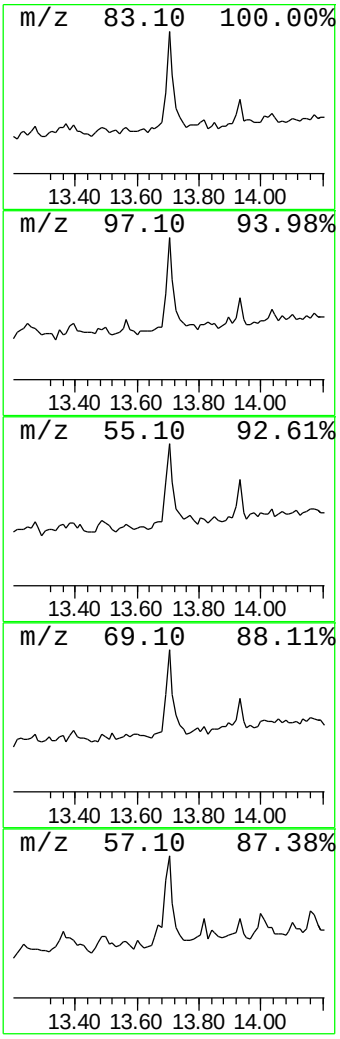
Peak Number 11 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	4.72 ng	122320	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	1-Nonadecene	266	C19H38	018435-45-5	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





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Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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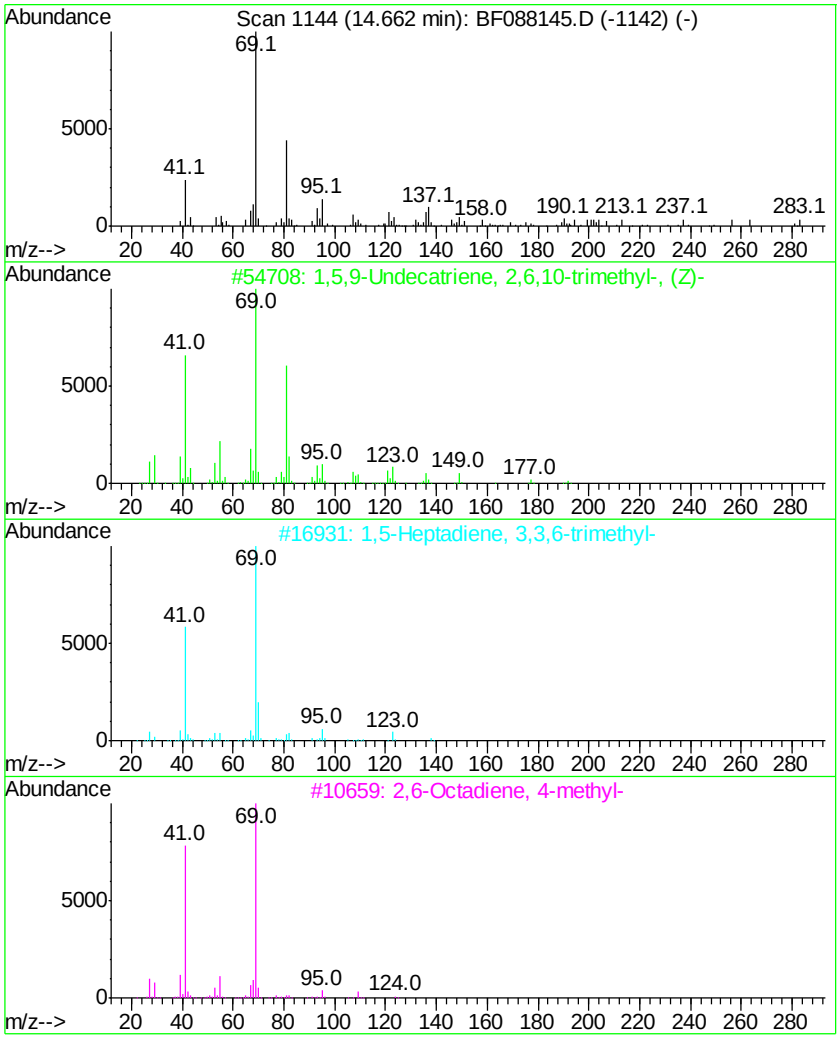
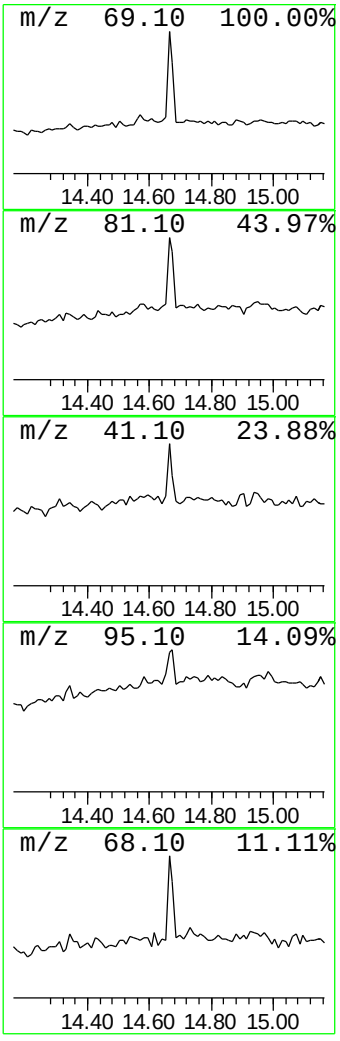
Peak Number 12 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.72 ng	53087	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
2	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53
3	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	50
4	Cyclopropanecarboxylic acid, 3,5...	190	C12H14O2	1000307-52-3	50
5	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	50





Tentatively Identified Compound (LSC) summary

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Data File : BF088145.D
Acq On : 18 Jun 2016 20:33
Operator : UM/SJ
Sample : H3580-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	1.87	2.2	ng	59550	1	6.68	531109	20.0
2-Pentanone, 4-hy...	4.84	3.6	ng	96800	1	6.68	531109	20.0
Octane, 3,6-dimet...	5.92	2.7	ng	71339	1	6.68	531109	20.0
unknown6.46	6.46	61.9	ng	1643150	1	6.68	531109	20.0
unknown7.34	7.34	2.2	ng	70914	2	7.98	637404	20.0
Octane, 2,6-dimet...	8.41	4.3	ng	136329	2	7.98	637404	20.0
Pentadecane, 2,6,...	10.38	3.3	ng	105033	3	9.72	632229	20.0
Tridecane	10.64	6.6	ng	174127	4	11.20	531227	20.0
Behenic alcohol	13.70	4.7	ng	122320	5	13.83	518432	20.0
1,5,9-Undecatrien...	14.66	2.7	ng	53087	6	15.21	390193	20.0