LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)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	18232	26405	1.36%	0.141%
2	1.781	15	17	24	rVV	153271	198127	10.22%	1.055%
3	1.884	24	26	34	rVB	42401	63884	3.30%	0.340%
4	4.844	283	285	290	rBV	77259	110629	5.71%	0.589%
5	4.913	290	291	294	rVB	18600	20067	1.04%	0.107%
6	5.290	321	324	326	rBV	1672635	1938246	100.00%	10.318%
7	5.667	355	357	360	rVB	13888	19490	1.01%	0.104%
8	5.873	373	375	378	rBV2	12690	21415	1.10%	0.114%
9	5.919	378	379	382	rVV2	30611	41365	2.13%	0.220%
10	6.342	413	416	419	rBV2	1610947	1819930	93.90%	9.688%
11	6.456	423	426	429	rVV	1866632	1770380	91.34%	9.425%
12	6.536	431	433	435	rVB	24026	33394	1.72%	0.178%
13	6.627	435	441	442	rBV4	18410	48957	2.53%	0.261%
14	6.685	444	446	450	rVB	639214	550879	28.42%	2.933%
15	6.753	450	452	453	rBV2	18088	31035	1.60%	0.165%
16	6.810	455	457	458	rVV	42802	50277	2.59%	0.268%
17	6.845	458	460	462	rVV	1557305	1634840	84.35%	8.703%
18	6.913	464	466	468	rVV3	14149	28804	1.49%	0.153%
19	6.959	468	470	473	rVV3	18836	35417	1.83%	0.189%
20	7.039	475	477	479	rBV2	14072	19556	1.01%	0.104%
21	7.107	481	483	487	rVV4	20301	51447	2.65%	0.274%
22	7.210	490	492	493	rVV2	19141	29579	1.53%	0.157%
23	7.256	493	496	498	rVV	1132867	1175394	60.64%	6.257%
24	7.325	500	502	506	rVV3	25870	71135	3.67%	0.379%
25	7.382	506	507	512	rVV	32632	51408	2.65%	0.274%
26	7.496	515	517	519	rVV	33513	37795	1.95%	0.201%
27	7.610	523	527	529	rVB3	24478	47659	2.46%	0.254%
28	7.725	535	537	541	rVB3	19532	37115	1.91%	0.198%
29	7.793	541	543	545	rBV	14615	21248	1.10%	0.113%
30	7.862	545	549	551	rBV3	10371	29063	1.50%	0.155%
31	7.976	556	559	561	rBV	516431	645819	33.32%	3.438%
32	8.102	566	570	572	rVB5	10408	27265	1.41%	0.145%
33	8.410	594	597	601	rVB2	53644	111338	5.74%	0.593%
34	8.662	618	619	621	rVB	18326	19898	1.03%	0.106%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)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	8.856	632	636	637	rBV3	15947	20522	1.06%	0.109%
36	9.005	646	649	650	rVB	54962	53947	2.78%	0.287%
37	9.051	650	653	655	rBV	1988854	1797941	92.76%	9.571%
38	9.131	657	660	663	rBV4	16582	40448	2.09%	0.215%
39	9.451	684	688	690	rBV	606375	597970	30.85%	3.183%
40	9.633	702	704	705	rVB	26552	21857	1.13%	0.116%
41	9.668	705	707	709	rBV	44319	40968	2.11%	0.218%
42	9.725	709	712	714	rVB	588652	635529	32.79%	3.383%
43	9.896	724	727	728	rBV	14996	28139	1.45%	0.150%
44	9.988	733	735	736	rVB	27729	23852	1.23%	0.127%
45	10.125	745	747	749	rBV2	14661	25676	1.32%	0.137%
46	10.159	749	750	752	rVB	68845	61278	3.16%	0.326%
47	10.376	766	769	772	rBV	45466	77705	4.01%	0.414%
48	10.514	778	781	783	rBV	748959	895797	46.22%	4.769%
49	10.594	786	788	790	rVV2	18003	27108	1.40%	0.144%
50	10.639	790	792	796	rVV2	75346	143770	7.42%	0.765%
51	10.834	806	809	813	rVB4	13851	34759	1.79%	0.185%
52	11.085	829	831	832	rBV	30954	46582	2.40%	0.248%
53	11.108	832	833	836	rVB	39842	38704	2.00%	0.206%
54	11.199	839	841	844	rVV	663792	563019	29.05%	2.997%
55	11.268	845	847	850	rVB3	13808	20376	1.05%	0.108%
56	11.805	892	894	899	rVB3	11143	25760	1.33%	0.137%
57	12.411	944	947	948	rBV	28897	32397	1.67%	0.172%
58	12.639	964	967	968	rBV	20208	28806	1.49%	0.153%
59	12.777	977	979	982	rBV	938241	1313242	67.75%	6.991%
60	13.360	1028	1030	1034	rBV4	11219	23547	1.21%	0.125%
61	13.702	1057	1060	1067	rVB	75722	144437	7.45%	0.769%
62	13.828	1068	1071	1077	rVV	570089	566420	29.22%	3.015%
63	13.931	1078	1080	1082	rVB	36427	37936	1.96%	0.202%
64	14.663	1142	1144	1146	rVB	62026	67271	3.47%	0.358%
65	14.937	1166	1168	1178	rVB7	26519	62503	3.22%	0.333%
66	15.211	1190	1192	1198	rBV	343034	401005	20.69%	2.135%
67	16.526	1304	1307	1314	rVB5	30084	66093	3.41%	0.352%

Sum of corrected areas: 18784624

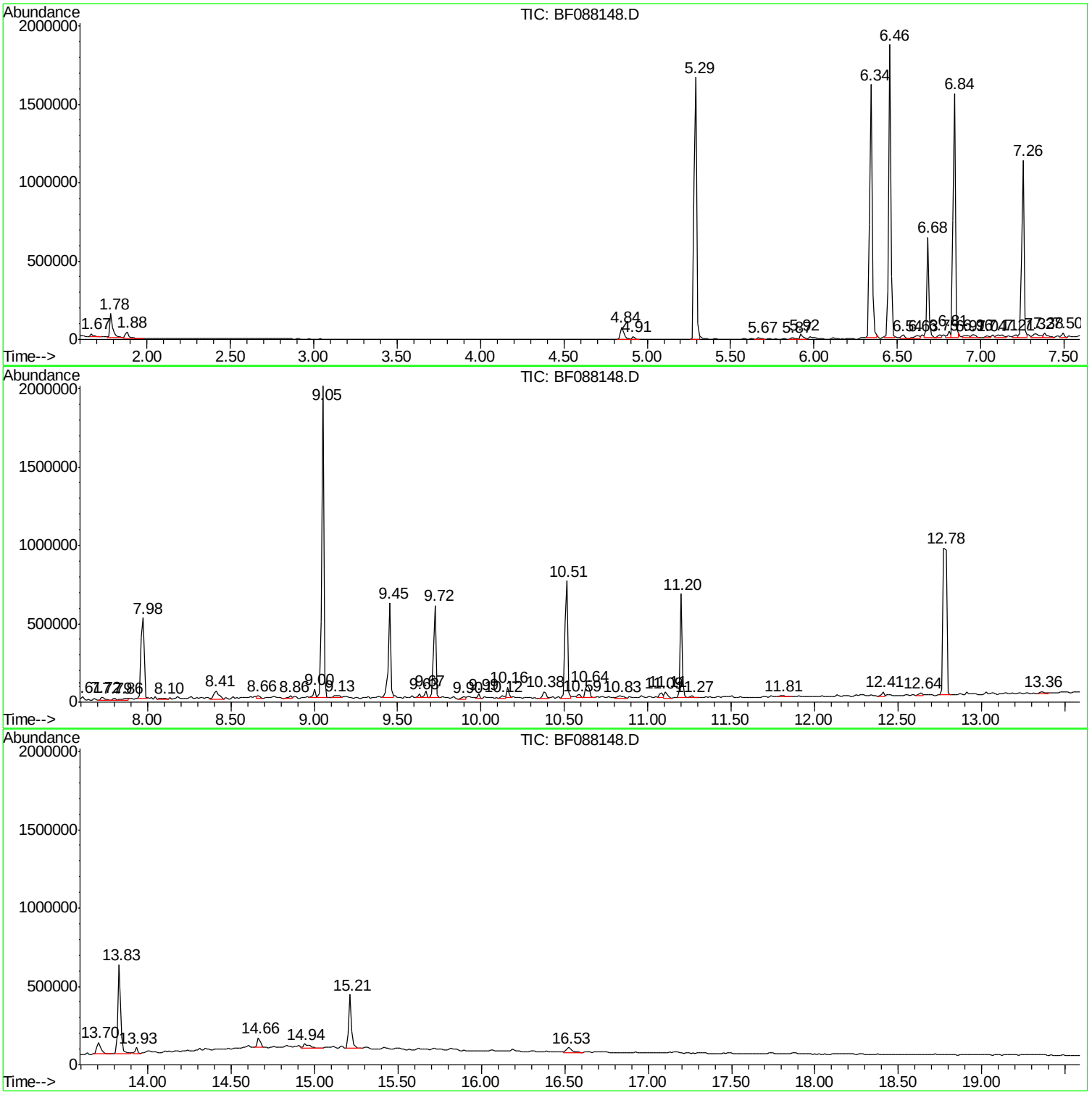
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)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 : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

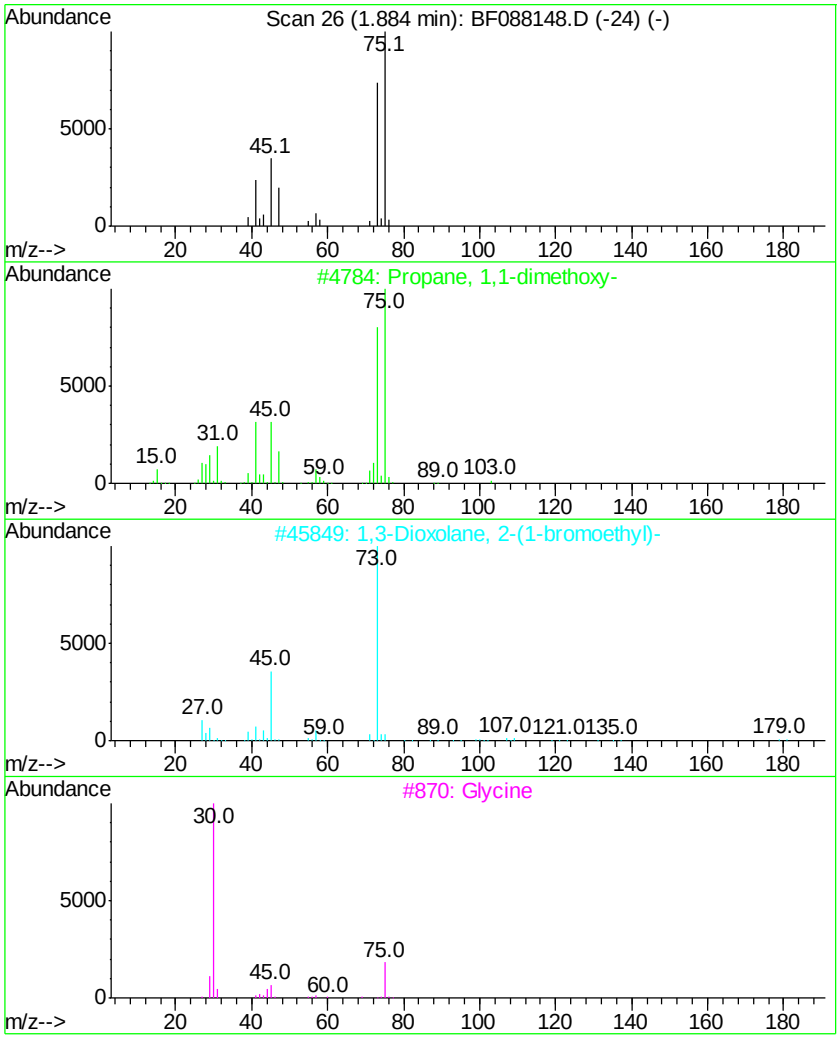
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

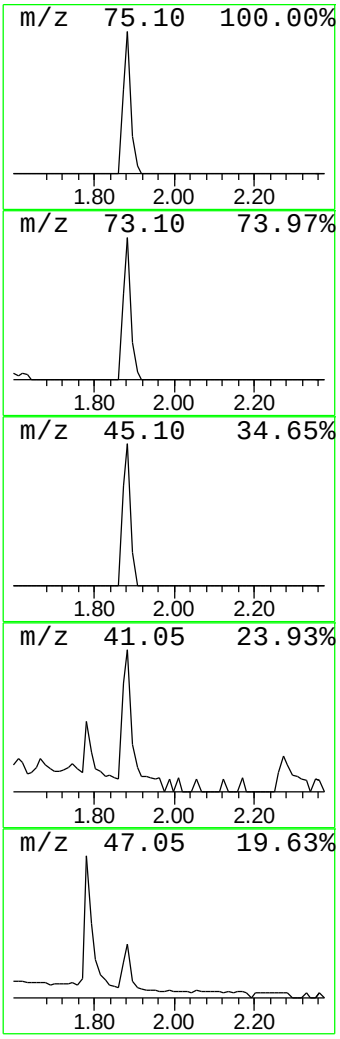
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.88	2.32 ng	63884	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	78
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
3	Glycine	75	C2H5NO2	000056-40-6	9
4	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)C

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

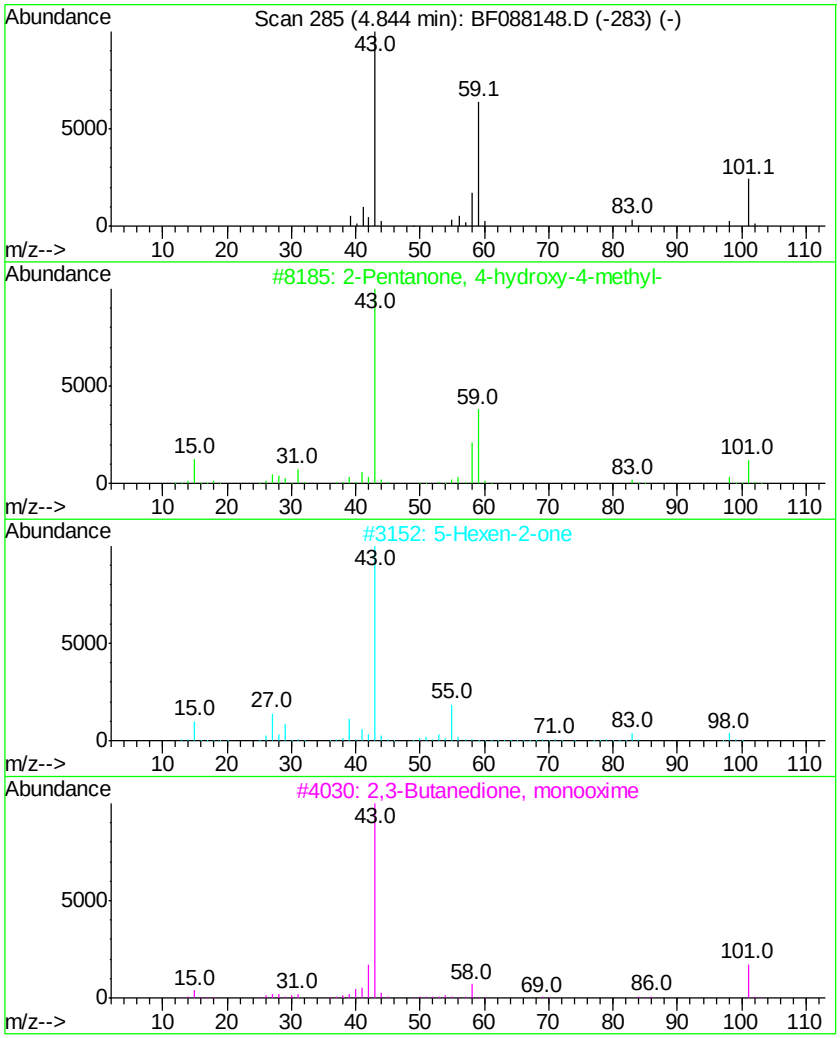
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

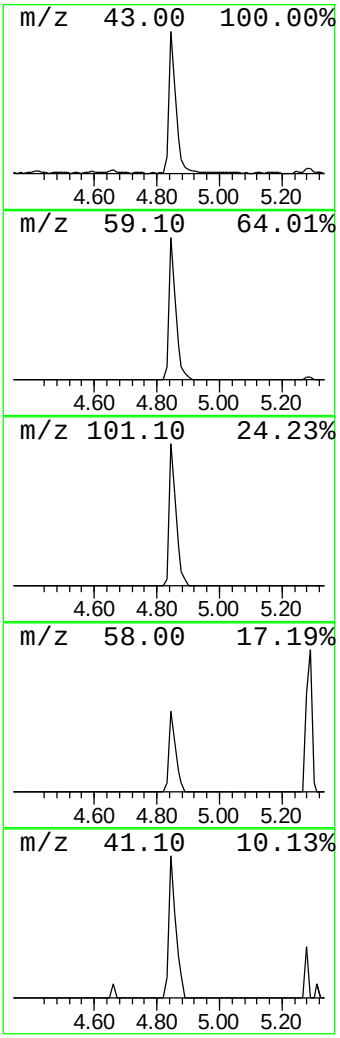
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	4.02 ng	110629	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	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	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





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)C

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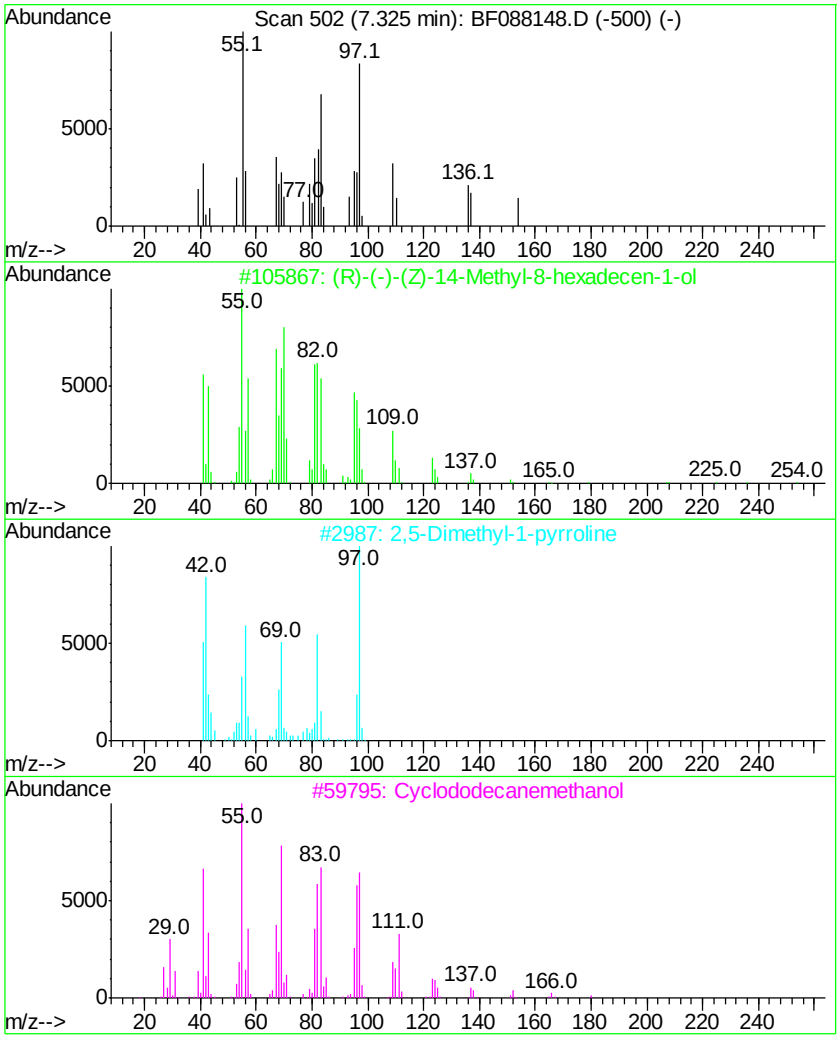
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

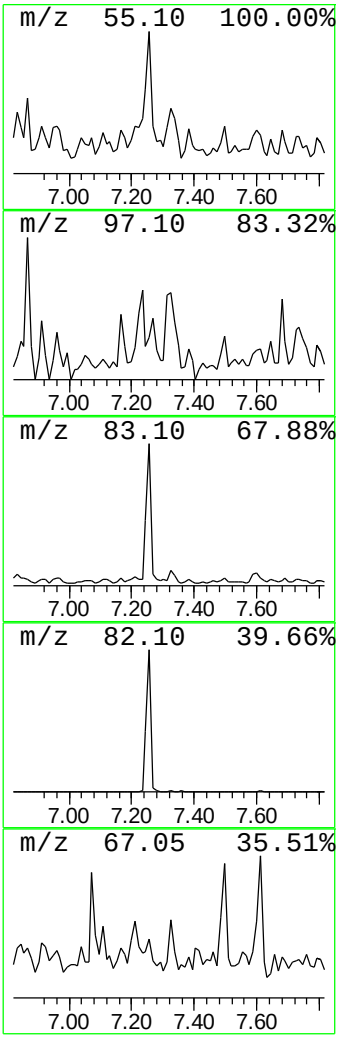
****

Peak Number 6 unknown7.32 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	2.58 ng	71135	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(-)-(Z)-14-Methyl-8-hexadece...	254	C17H34O	030689-78-2	43
2	2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	38
3	Cyclododecanemethanol	198	C13H26O	001892-12-2	38
4	Z-10-Pentadecen-1-ol	226	C15H30O	1000245-48-5	35
5	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)C

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

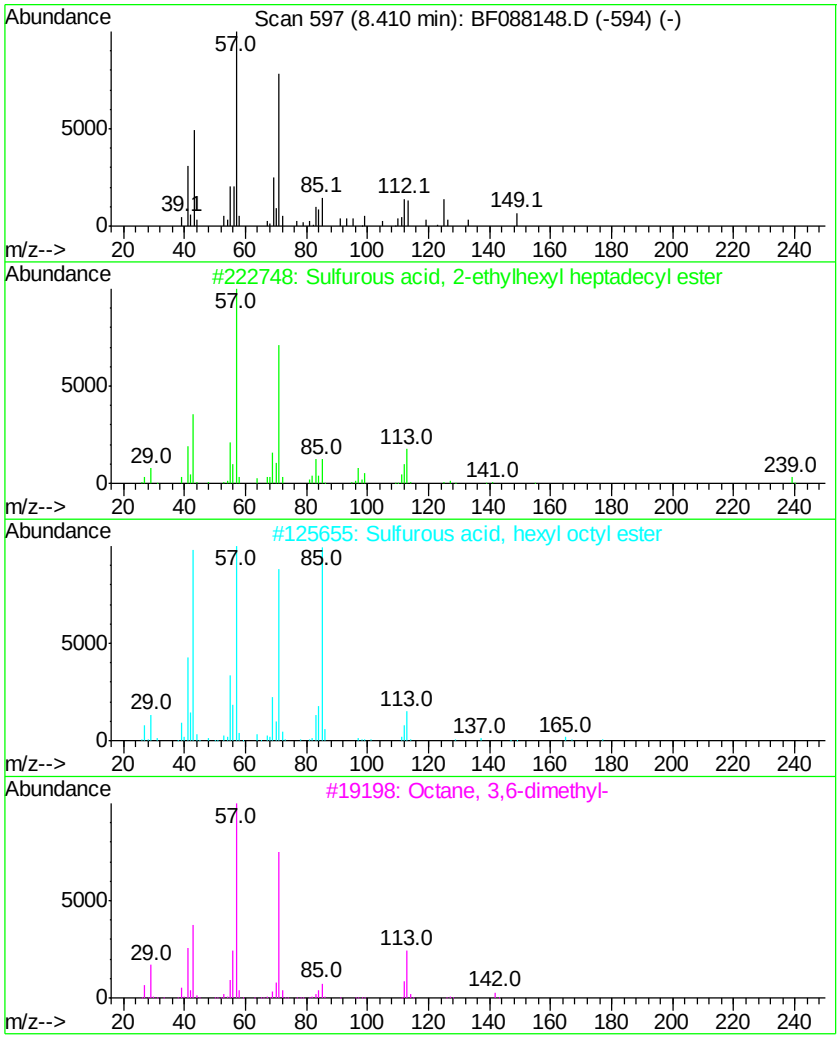
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

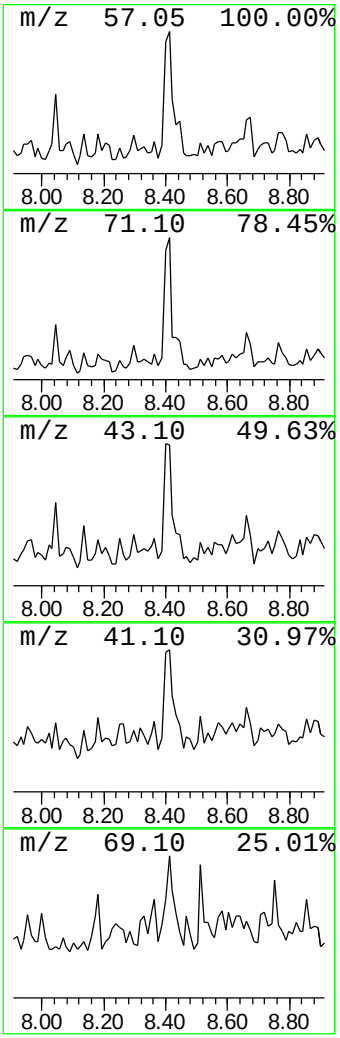
****

Peak Number 7 Sulfurous acid, 2-ethylhexy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	3.45 ng	111338	Naphthalene-d8	7.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	72
2	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	64
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
4	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	64
5	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)C

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

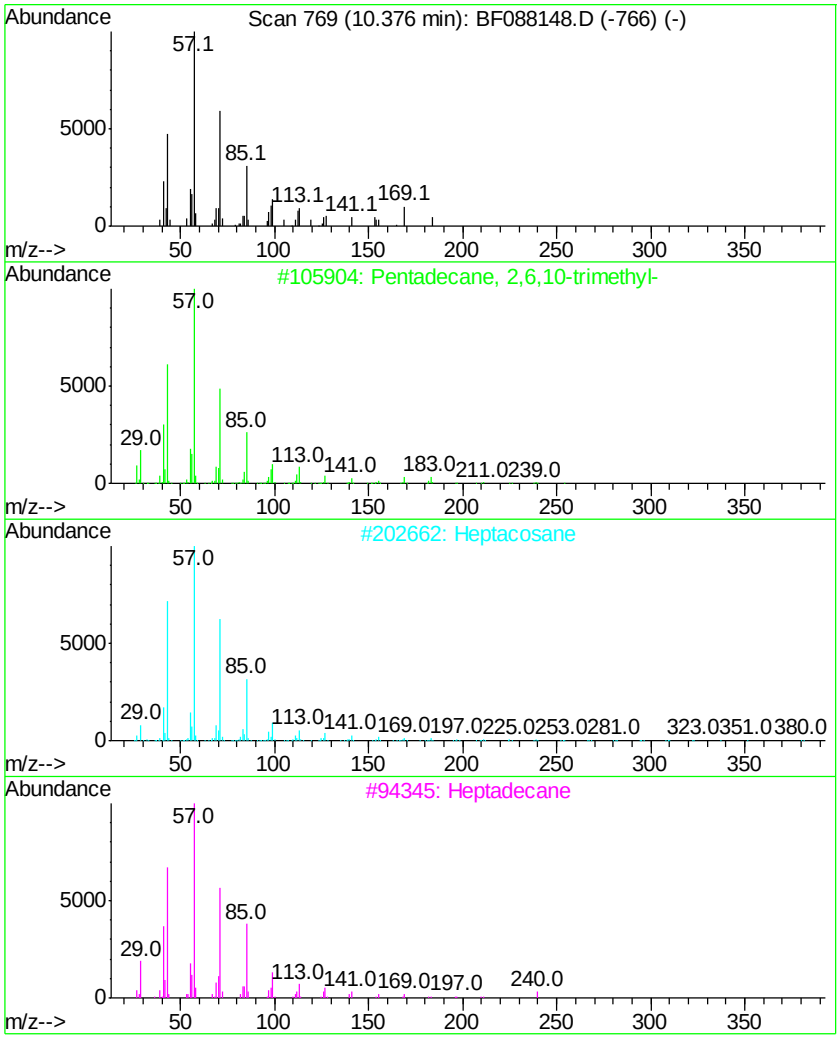
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

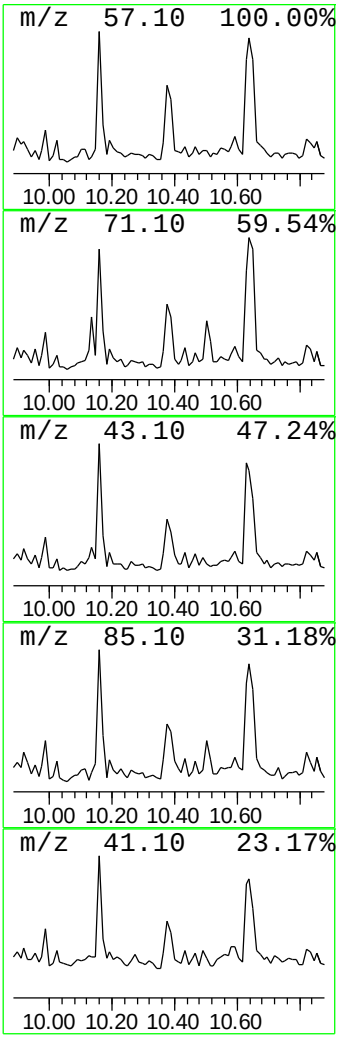
****

Peak Number 8 Pentadecane, 2,6,10-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.45 ng	77705	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	80
2	Heptacosane	380	C27H56	000593-49-7	72
3	Heptadecane	240	C17H36	000629-78-7	72
4	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	68
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)C

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

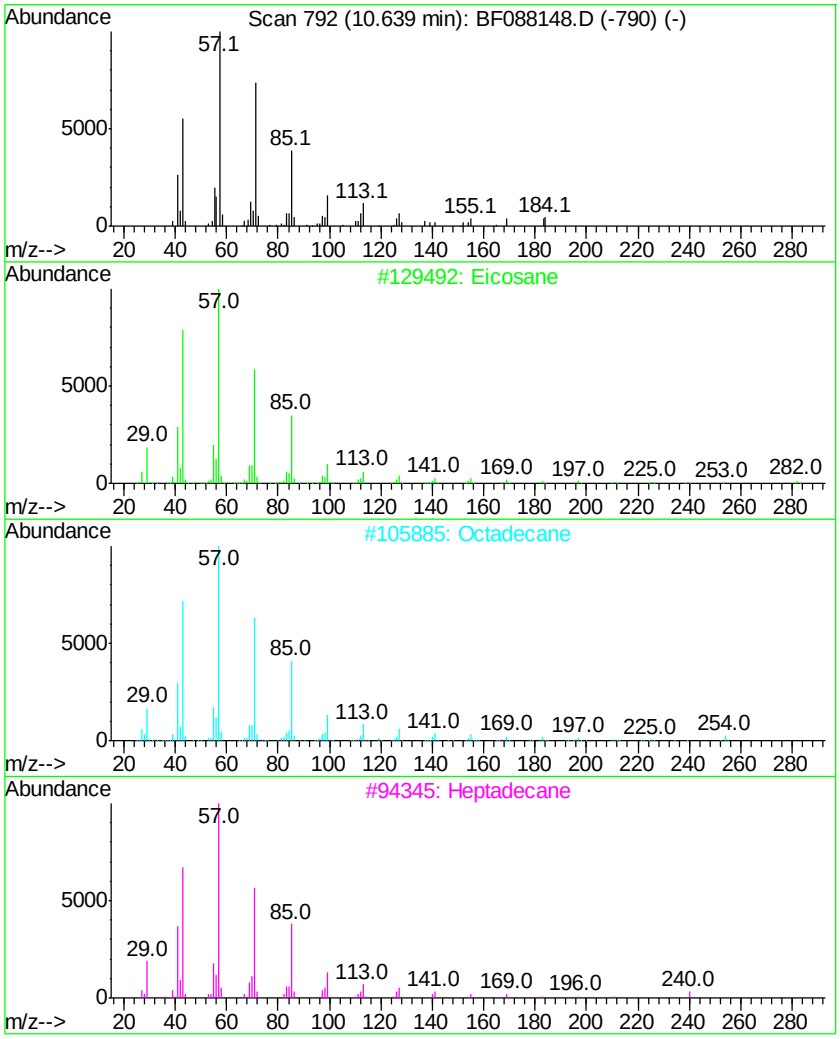
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

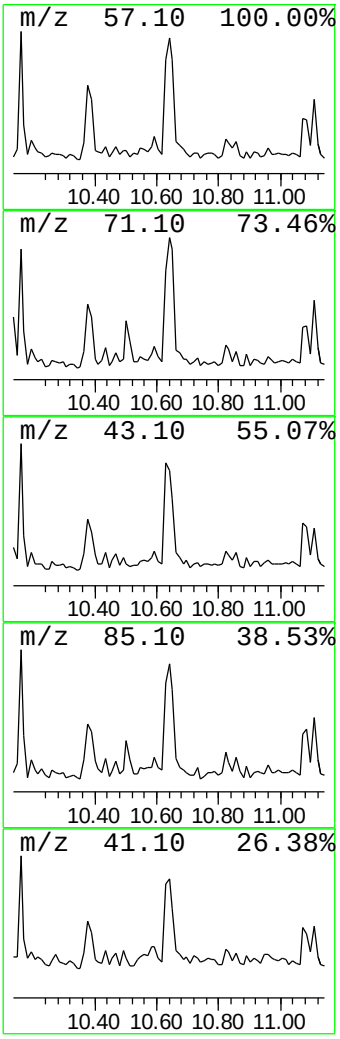
****

Peak Number 9 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	5.11 ng	143770	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Octadecane	254	C18H38	000593-45-3	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)C

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

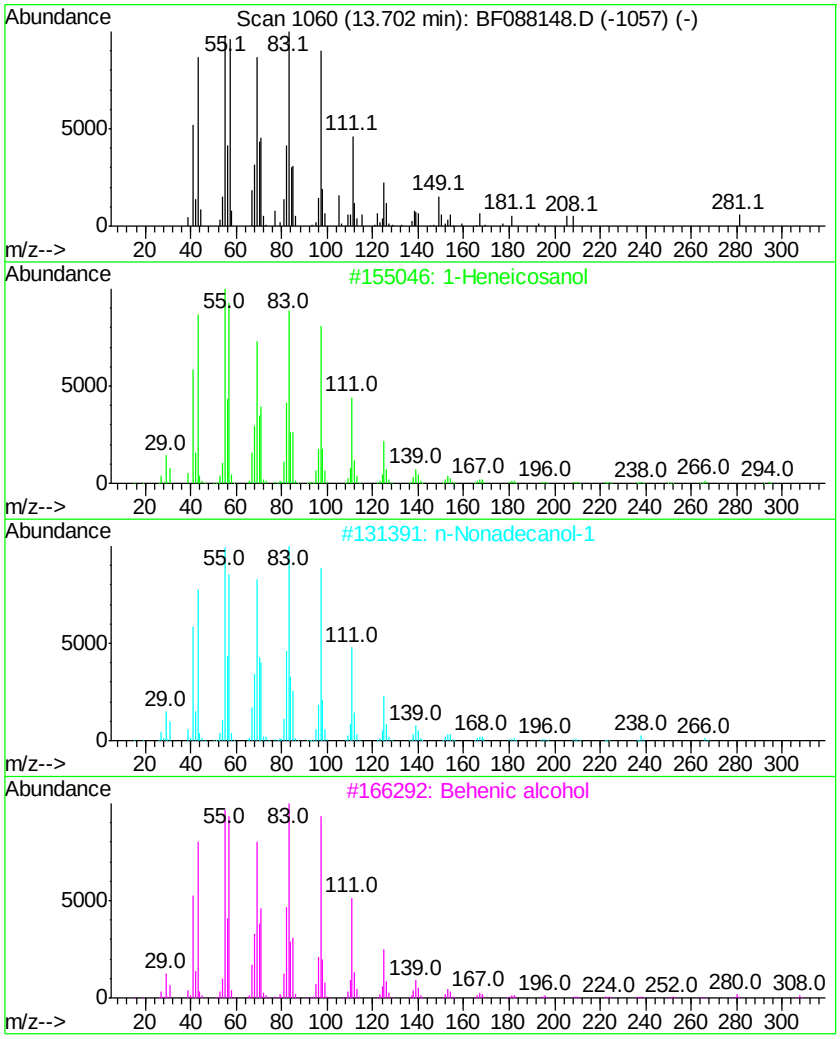
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

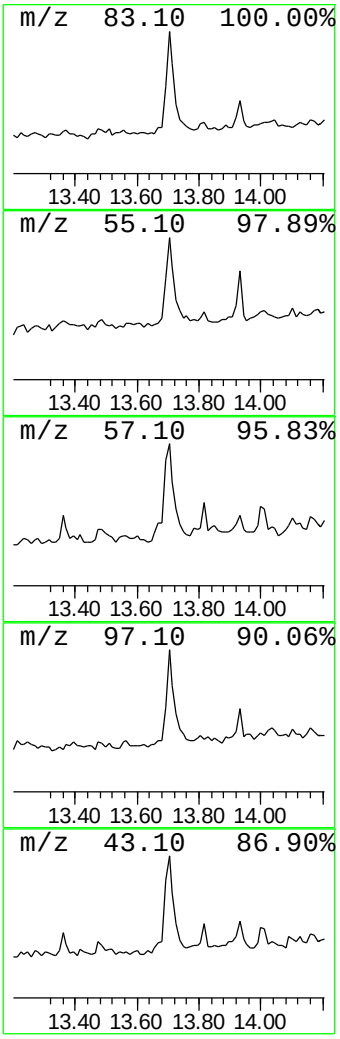
****

Peak Number 10 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	5.10 ng	144437	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)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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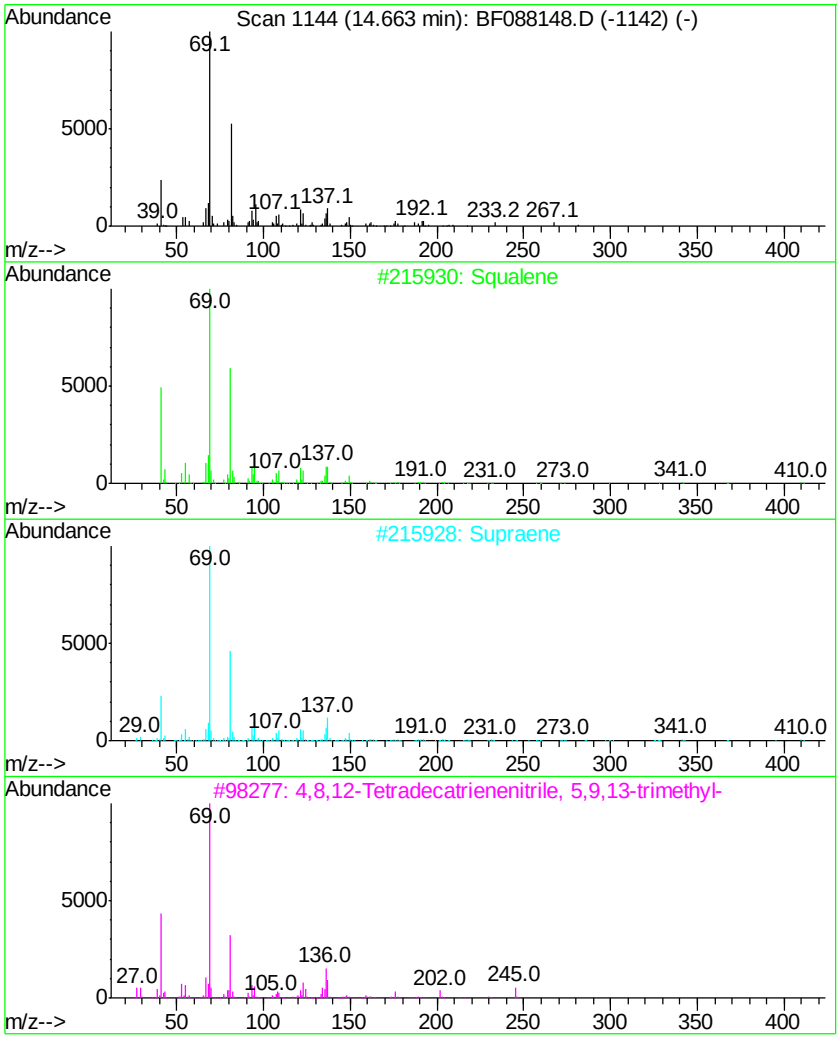
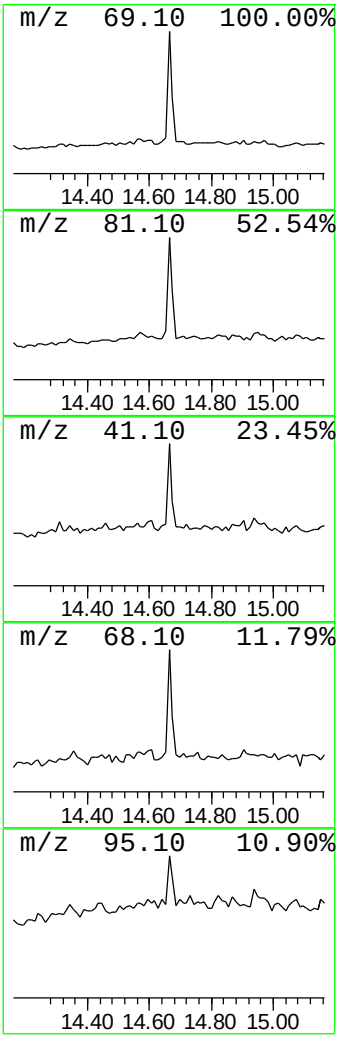
Peak Number 11 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.36 ng	67271	Perylene-d12	15.21

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	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	72
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64
5	3-Ethyl-1,5-octadiene	138	C10H18	1000114-87-7	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)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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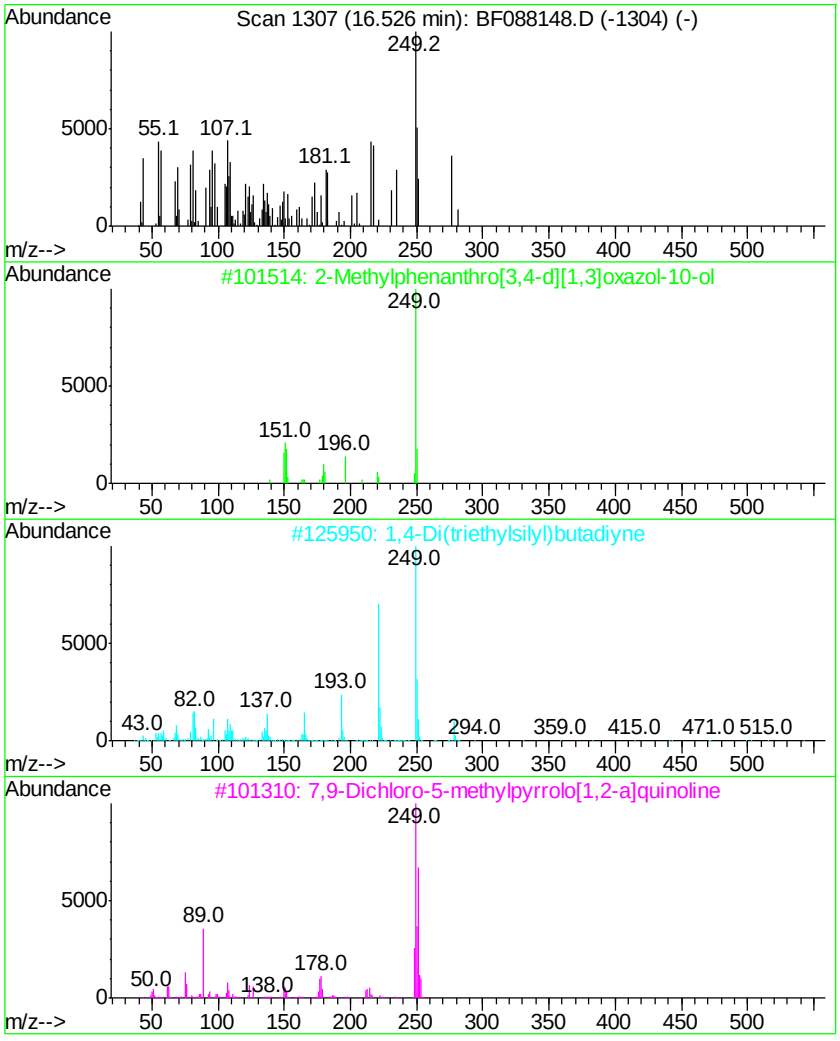
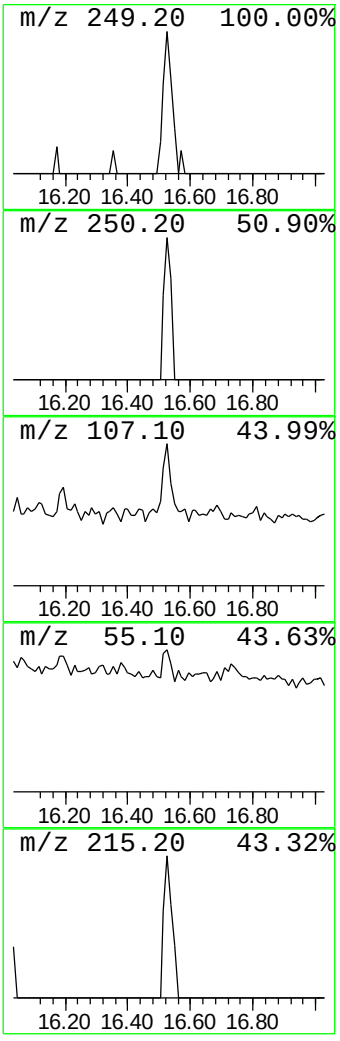
Peak Number 13 unknown16.53 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	3.30 ng	66093	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylphenanthro[3,4-d][1,3]ox...	249	C16H11NO2	098033-24-0	14
2	1,4-Di(triethylsilyl)butadiyne	278	C16H30Si2	1000334-26-4	14
3	7,9-Dichloro-5-methylpyrrolo[1,2...	249	C13H9Cl2N	1000251-52-9	14
4	1H-Pyrazole-3-acetic acid, 1-(4-...	250	C12H11FN2O3	1000338-24-4	10
5	Methyl 6-methylthio-4[1H]quinolo...	249	C12H11NO3S	1000255-48-3	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088148.D
Acq On : 18 Jun 2016 21:59
Operator : UM/SJ
Sample : H3580-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B6(8-16)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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	1.88	2.3	ng	63884	1	6.68	550879	20.0
2-Pentanone, 4-hy...	4.84	4.0	ng	110629	1	6.68	550879	20.0
unknown7.32	7.32	2.6	ng	71135	1	6.68	550879	20.0
Sulfurous acid, 2...	8.41	3.5	ng	111338	2	7.98	645819	20.0
Pentadecane, 2,6,...	10.38	2.5	ng	77705	3	9.72	635529	20.0
Eicosane	10.64	5.1	ng	143770	4	11.20	563019	20.0
1-Heneicosanol	13.70	5.1	ng	144437	5	13.83	566420	20.0
Squalene	14.66	3.4	ng	67271	6	15.21	401005	20.0
unknown16.53	16.53	3.3	ng	66093	6	15.21	401005	20.0