LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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	1.724	10	12	30	rVB	1068764	1996274	78.44%	10.116%
2	4.730	273	275	285	rBV	30999	66120	2.60%	0.335%
3	5.187	314	315	351	rBV7	428769	900763	35.39%	4.564%
4	6.262	408	409	416	rBV	386124	597687	23.49%	3.029%
5	6.364	416	418	431	rVB	1237802	1525393	59.94%	7.730%
6	6.593	436	438	444	rBV	471743	507649	19.95%	2.572%
7	6.753	450	452	454	rBV	1344573	1742316	68.46%	8.829%
8	7.176	486	489	491	rBV	976915	1403045	55.13%	7.110%
9	7.885	549	551	563	rBV	557971	685971	26.95%	3.476%
10	8.959	642	645	648	rBV	2353567	2544968	100.00%	12.896%
11	9.359	678	680	684	rBV	29527	36401	1.43%	0.184%
12	9.622	701	703	706	rBV	619193	787883	30.96%	3.992%
13	10.068	740	742	744	rVB	36338	30799	1.21%	0.156%
14	10.308	758	763	767	rBV2	25374	49762	1.96%	0.252%
15	10.422	770	773	775	rBV	1003789	1248178	49.04%	6.325%
16	10.502	778	780	782	rVV	84584	91275	3.59%	0.463%
17	10.536	782	783	786	rVB	33906	33546	1.32%	0.170%
18	10.593	786	788	790	rBV	46848	60729	2.39%	0.308%
19	11.108	831	833	835	rBV	708651	768709	30.21%	3.895%
20	11.714	884	886	888	rVB	104375	105202	4.13%	0.533%
21	11.862	898	899	906	rBV	23338	34152	1.34%	0.173%
22	12.514	954	956	959	rBV2	291387	331538	13.03%	1.680%
23	12.594	962	963	965	rVB	93702	70910	2.79%	0.359%
24	12.685	968	971	974	rBV	2019072	2079146	81.70%	10.535%
25	12.925	989	992	993	rBV	25063	26281	1.03%	0.133%
26	13.222	1015	1018	1020	rBV	179460	196908	7.74%	0.998%
27	13.268	1020	1022	1023	rBV	42593	67664	2.66%	0.343%
28	13.542	1042	1046	1048	rVV2	19662	40466	1.59%	0.205%
29	13.588	1048	1050	1055	rVB2	83621	104783	4.12%	0.531%
30	13.725	1060	1062	1065	rBV	559639	639033	25.11%	3.238%
31	13.908	1075	1078	1080	rBV	61915	77917	3.06%	0.395%
32	14.205	1102	1104	1107	rBV	64581	64902	2.55%	0.329%
33	14.502	1127	1130	1132	rBV	67303	75959	2.98%	0.385%
34	14.788	1153	1155	1157	rVB	56391	56993	2.24%	0.289%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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	15.085	1179	1181	1187	rVB	412955	561643	22.07%	2.846%
36	15.463	1212	1214	1218	rBV	29486	43113	1.69%	0.218%
37	15.885	1248	1251	1253	rVB	21555	38526	1.51%	0.195%
38	16.777	1326	1329	1335	rBV5	15625	42074	1.65%	0.213%

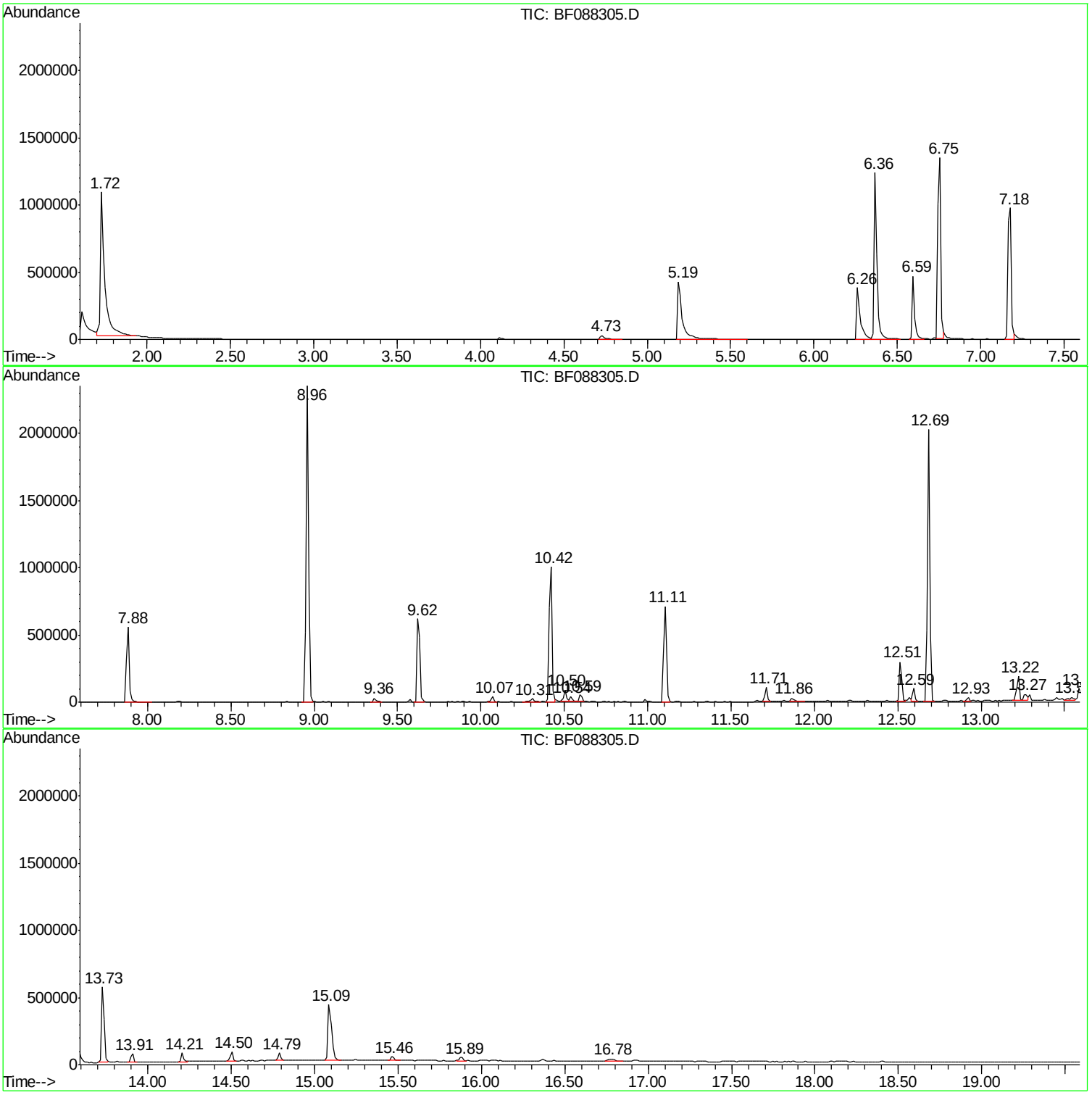
Sum of corrected areas: 19734678

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P0-002

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\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
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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

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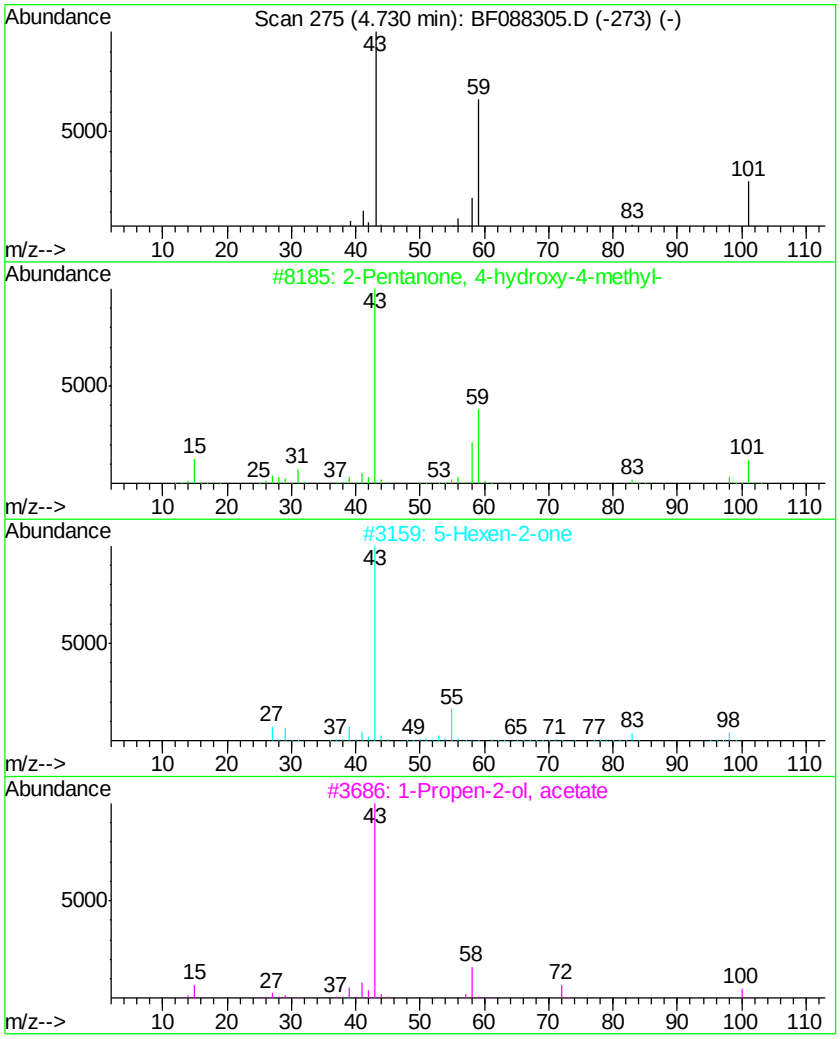
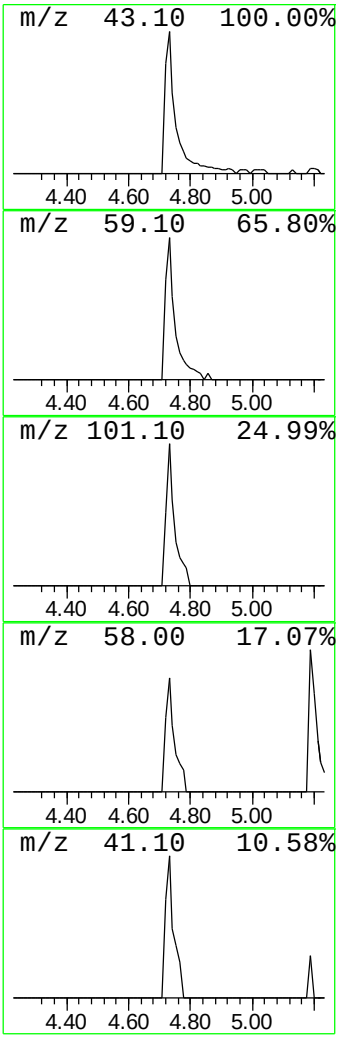
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	2.60 ng	66120	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	3-Hexanol	102	C6H14O	000623-37-0	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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

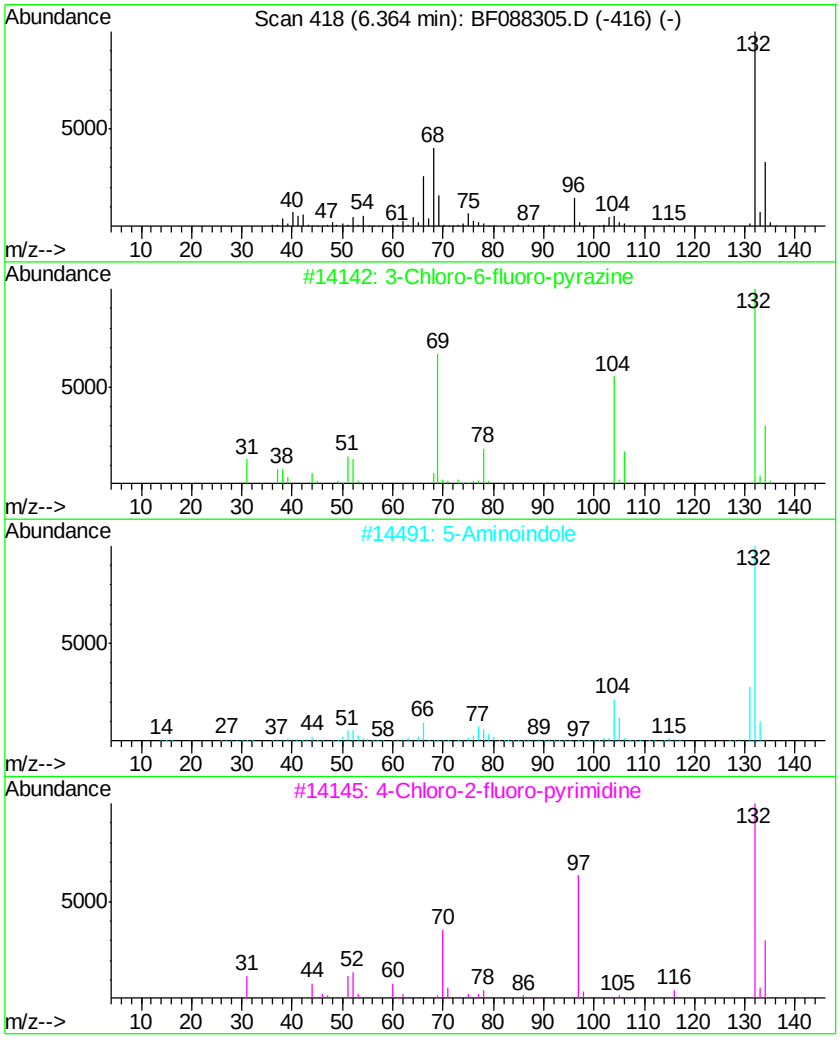
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

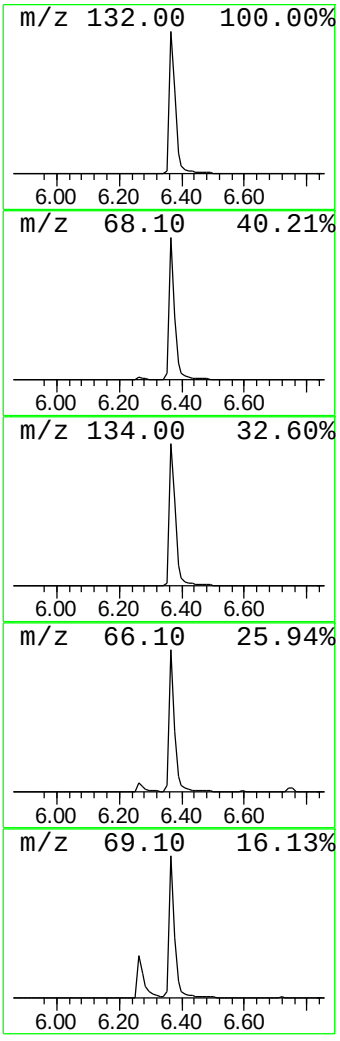
****

Peak Number 3 unknown6.36 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	60.10 ng	1525390	1,4-Dichlorobenzene-d4	6.59

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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
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Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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

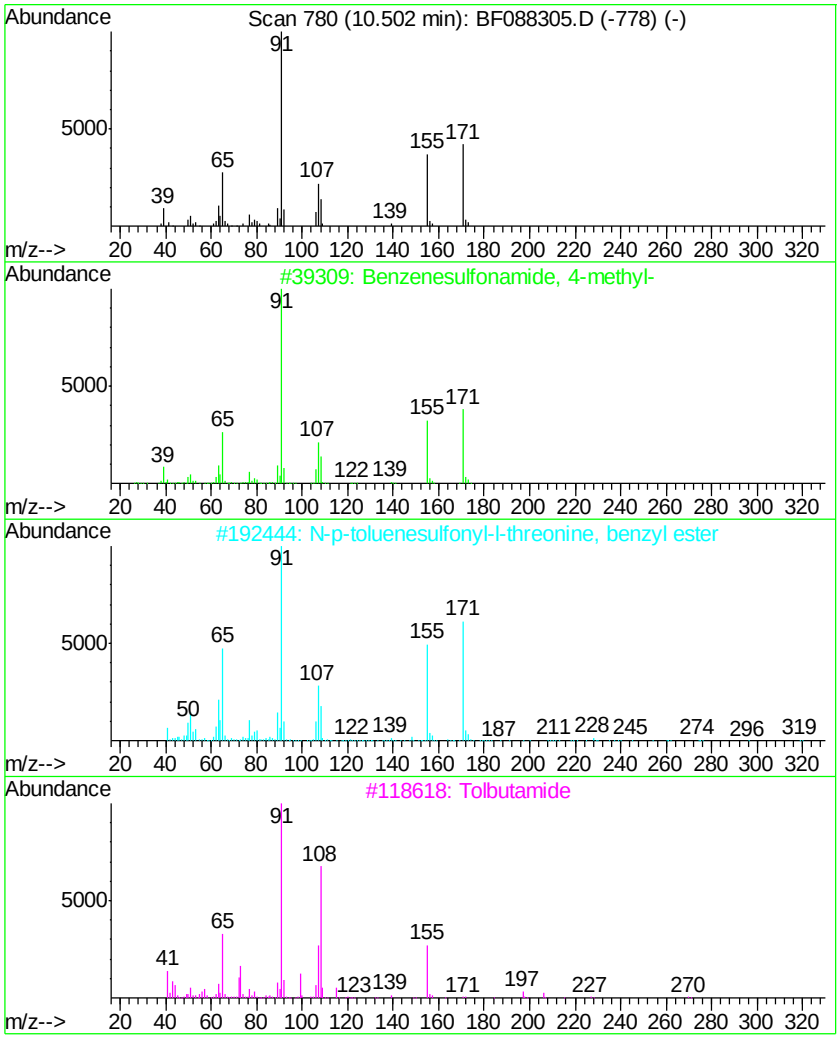
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

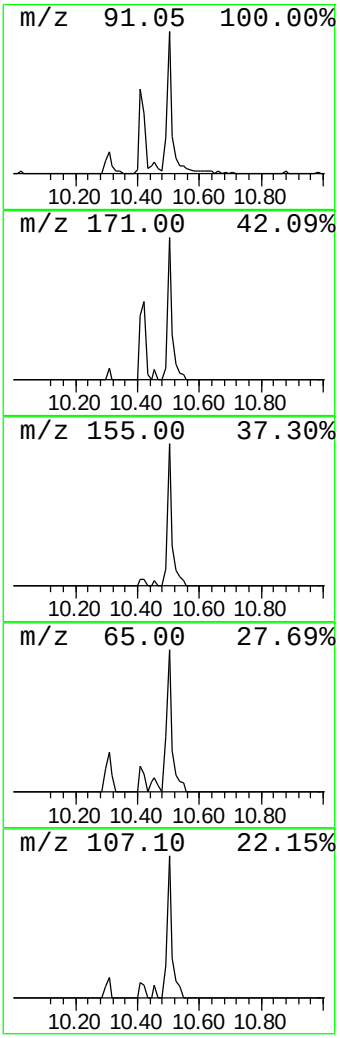
****

Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	2.37 ng	91275	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	74
3	Tolbutamide	270	C12H18N2O3S	000064-77-7	47
4	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	43
5	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	35





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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

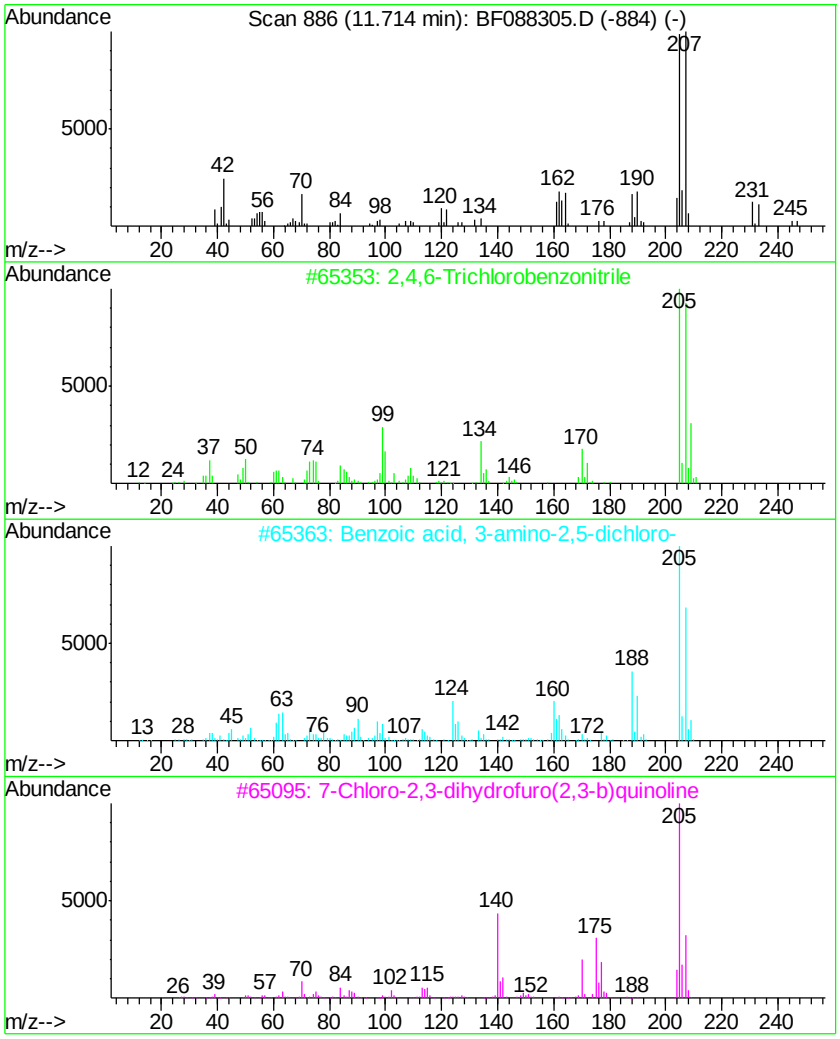
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

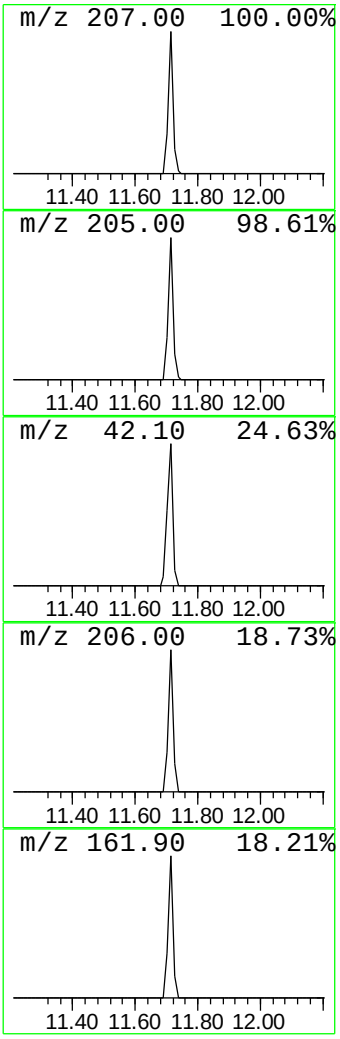
****

Peak Number 6 2,4,6-Trichlorobenzonitrile Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	2.74 ng	105202	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	53
2	Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	50
3	7-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-91-0	38
4	5-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-92-1	38
5	1,2,3,6-Tetrahydropyridine, 4-[4...	205	C12H15NO2	090684-19-8	35





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Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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

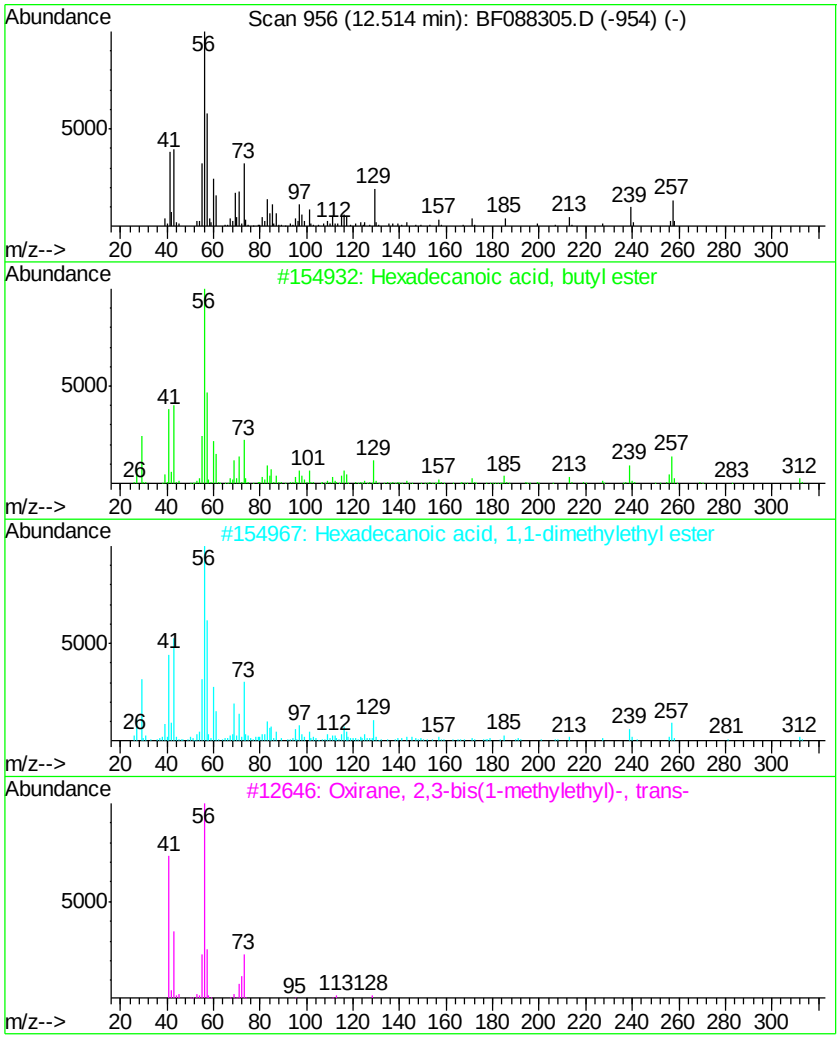
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

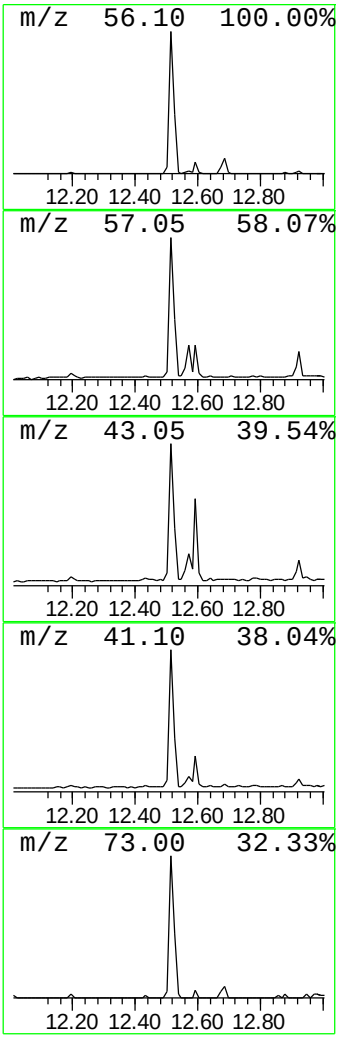
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	10.38 ng	331538	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
4	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35
5	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35





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Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
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Instrument : BNA_F
ClientSampleId : P0-002

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

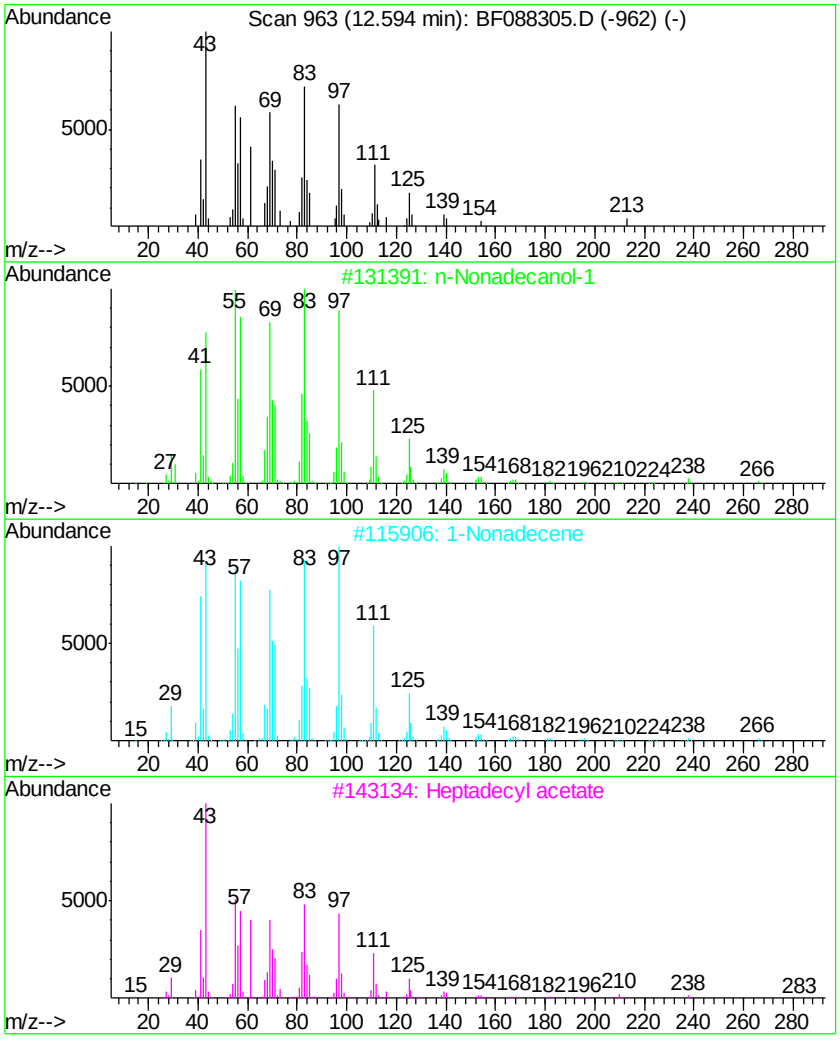
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

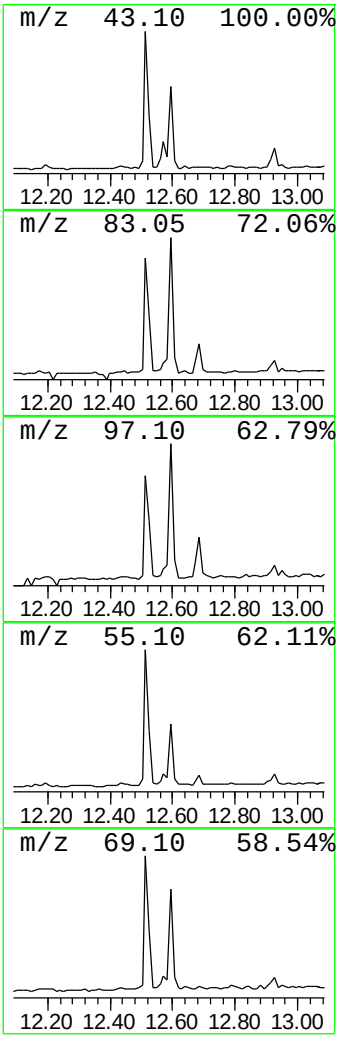
****

Peak Number 8 n-Nonadecanol-1 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	2.22 ng	70910	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2	1-Nonadecene	266	C19H38	018435-45-5	93
3	Heptadecyl acetate	298	C19H38O2	000822-20-8	91
4	1-Hexadecanol, acetate	284	C18H36O2	000629-70-9	91
5	1-Pentadecanol acetate	270	C17H34O2	000629-58-3	91





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Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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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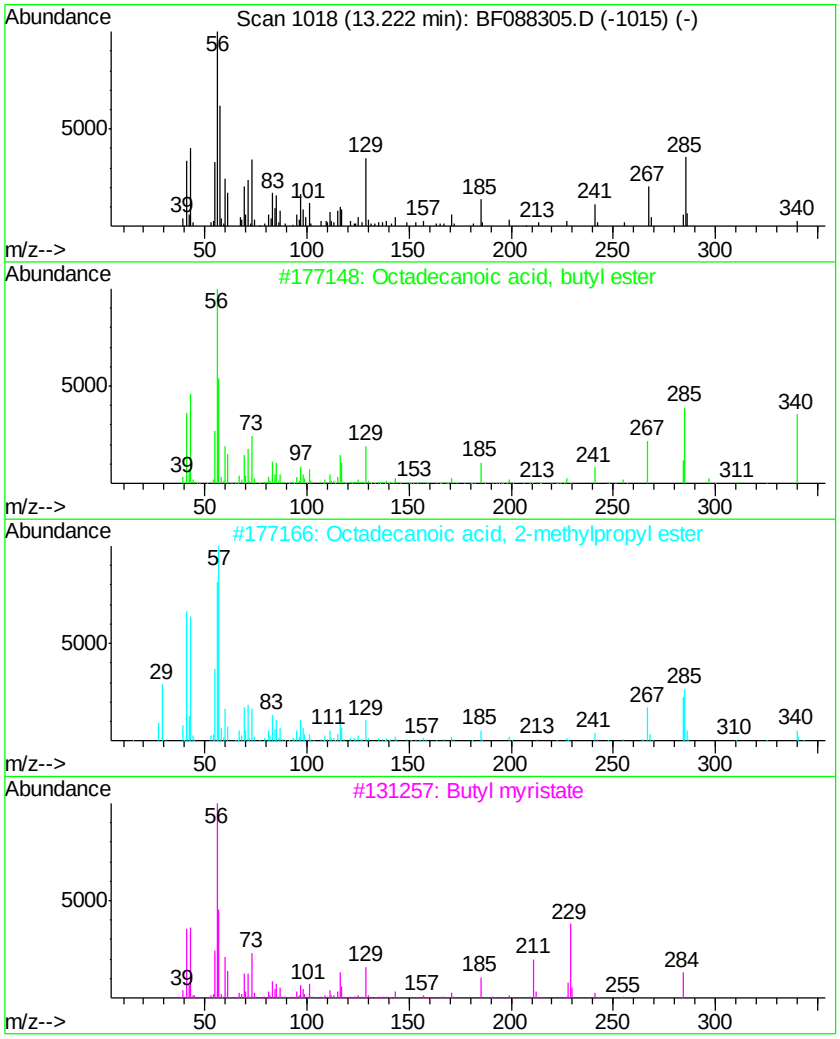
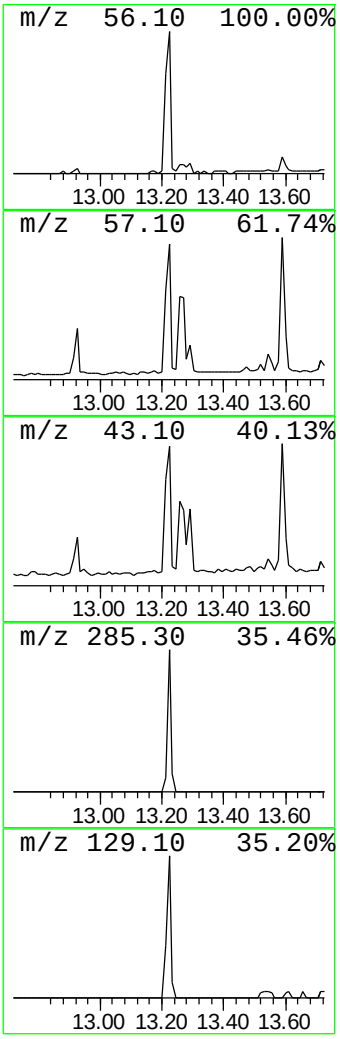
Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.22	6.16 ng	196908	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	83
3	Butyl myristate	284	C18H36O2	000110-36-1	47
4	Nipecotic acid	129	C6H11NO2	000498-95-3	43
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30





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Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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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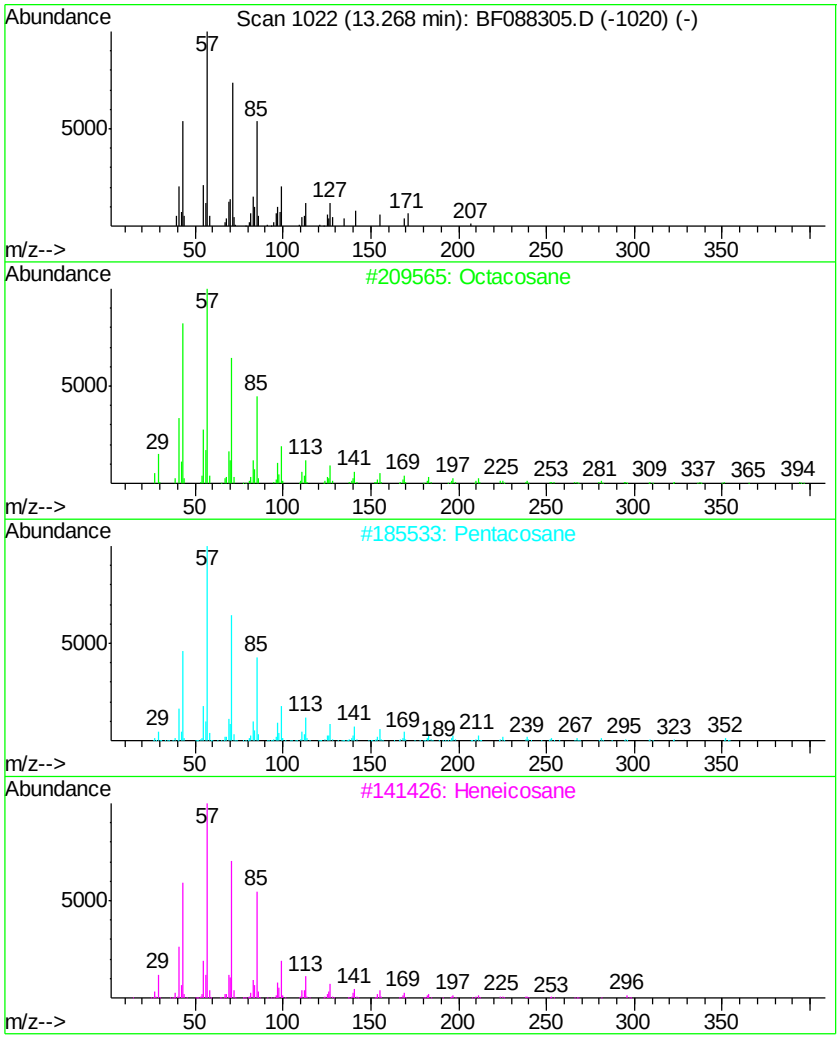
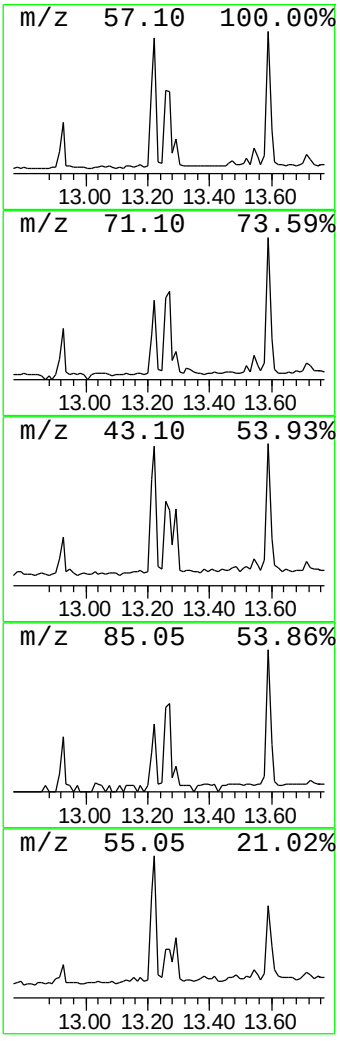
Peak Number 10 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	2.12 ng	67664	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Octadecane	254	C18H38	000593-45-3	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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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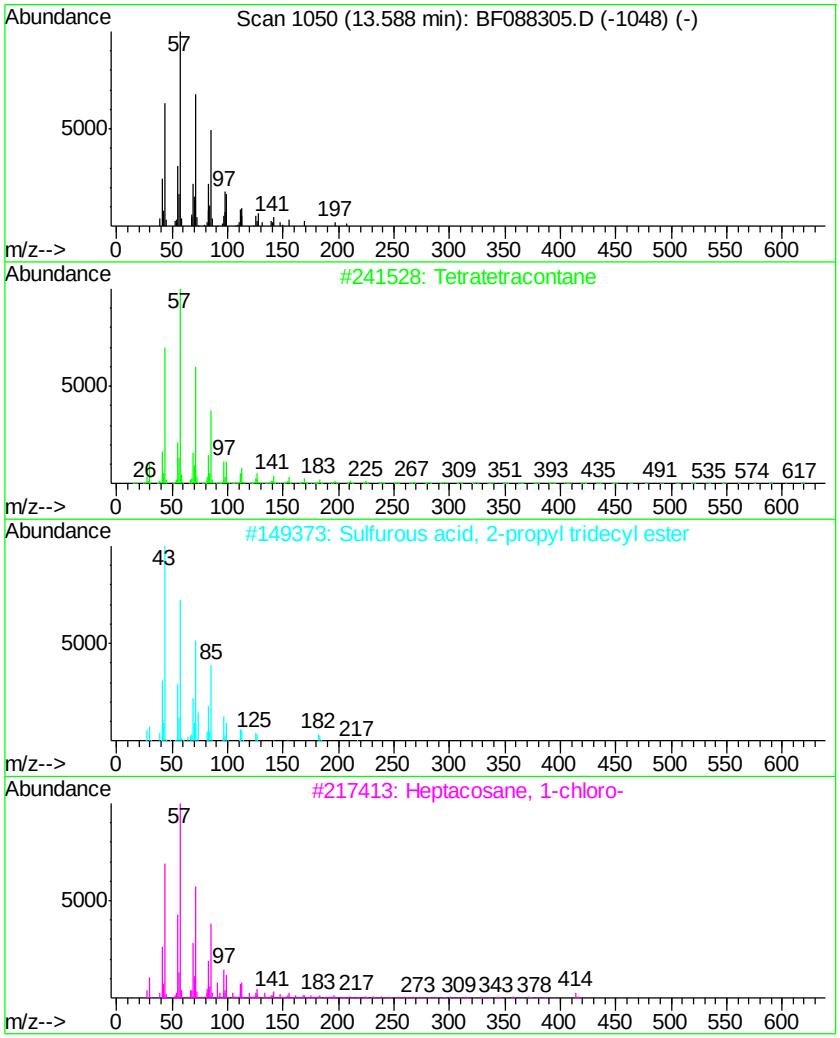
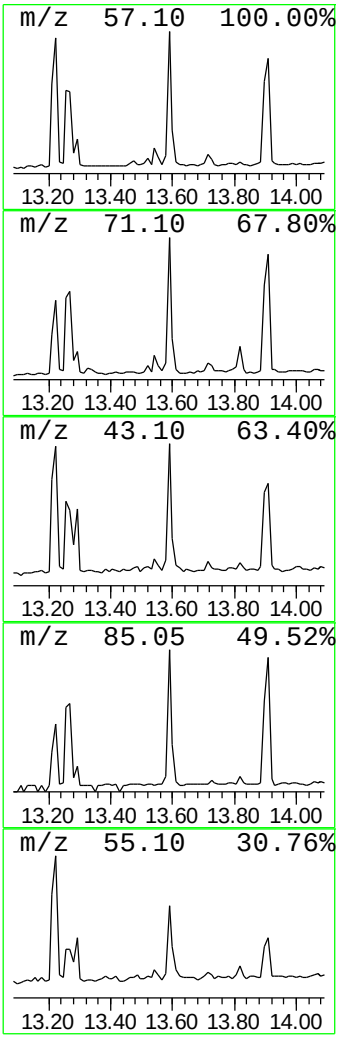
Peak Number 11 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	3.28 ng	104783	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
4	Tritetracontane	605	C43H88	007098-21-7	91
5	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	90





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Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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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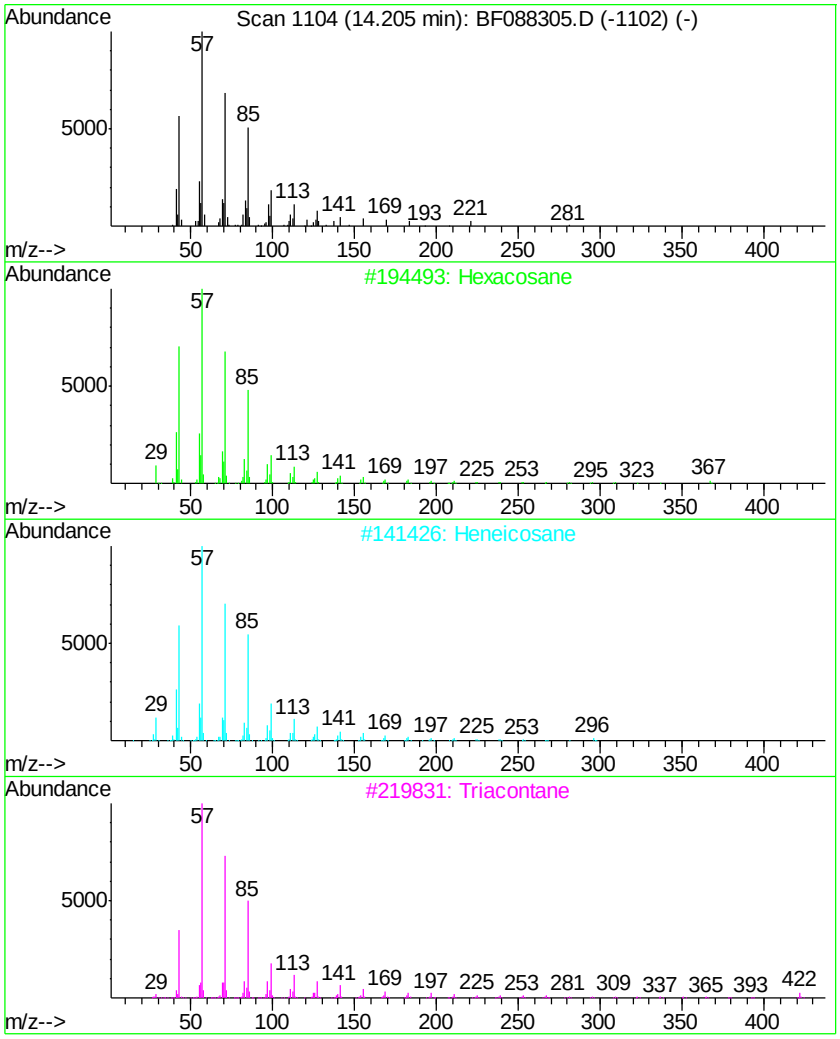
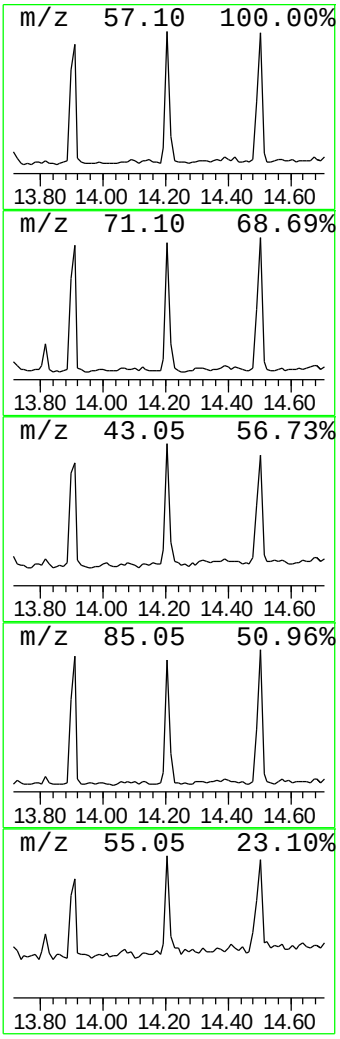
Peak Number 13 Hexacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	2.03 ng	64902	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Octacosane	394	C28H58	000630-02-4	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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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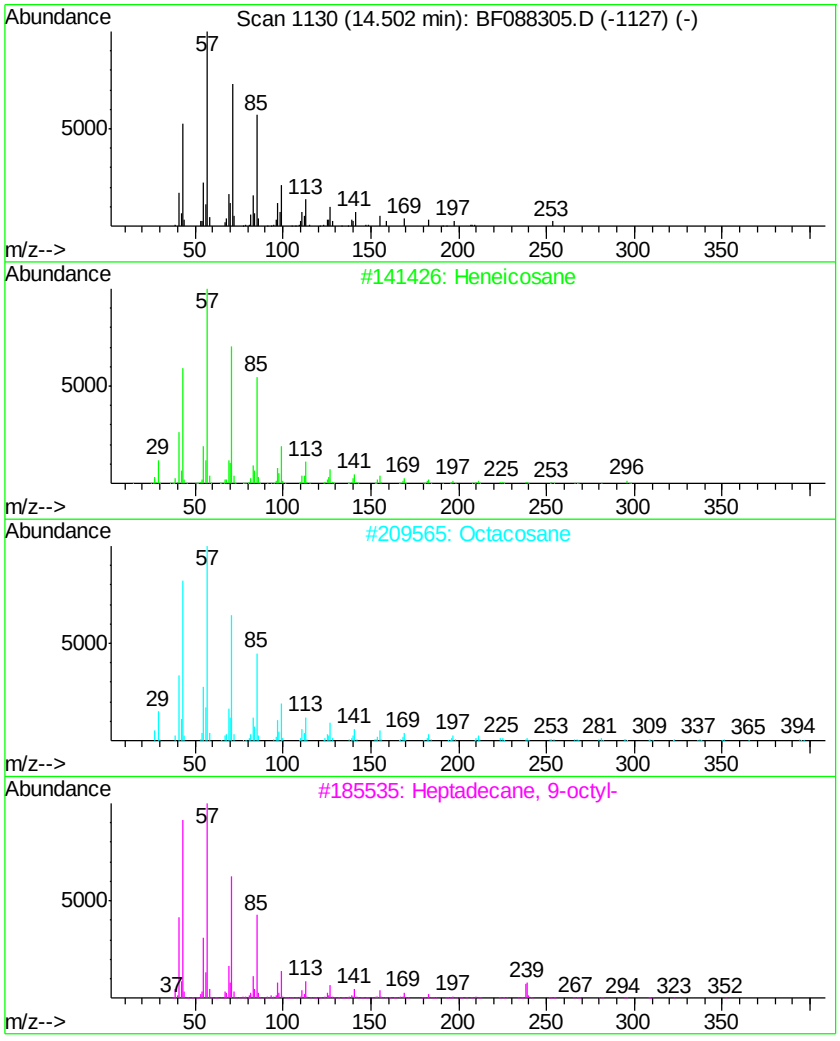
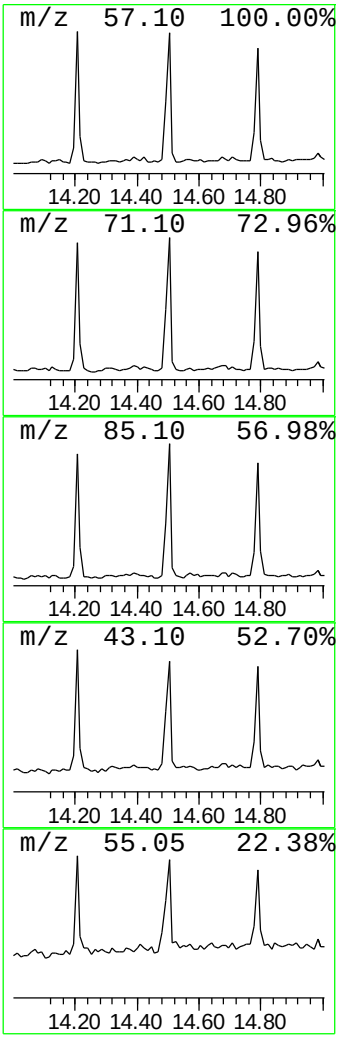
Peak Number 14 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	2.70 ng	75959	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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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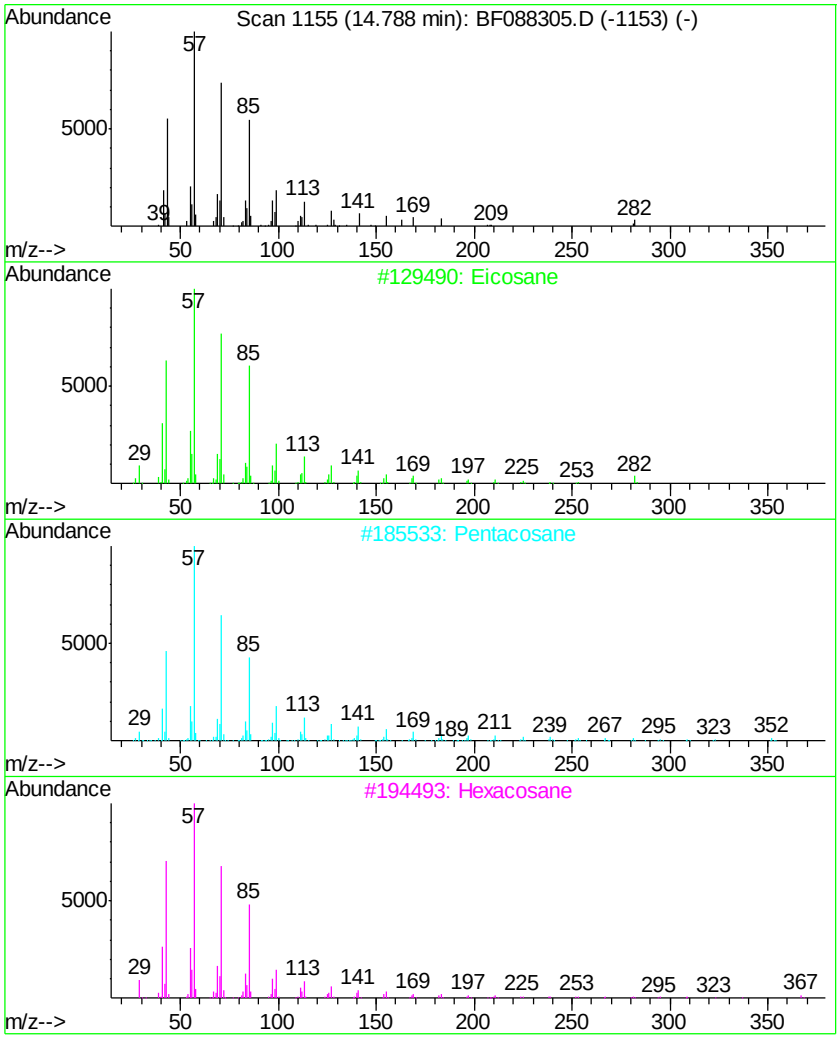
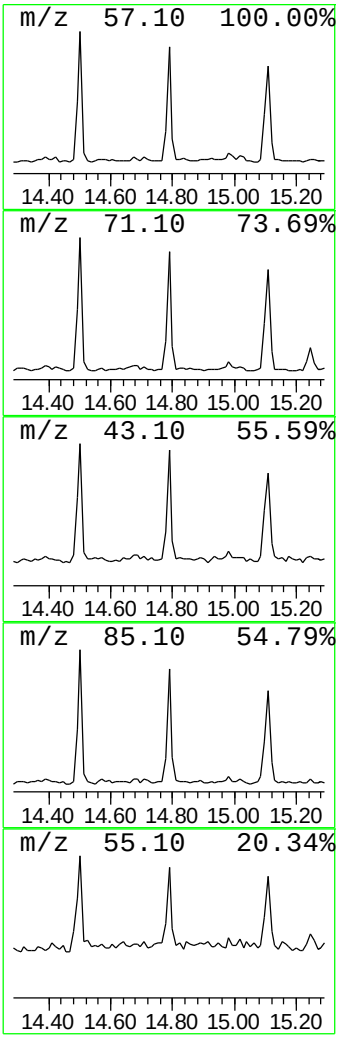
Peak Number 15 Eicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.03 ng	56993	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Pentacosane	352	C25H52	000629-99-2	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Octacosane	394	C28H58	000630-02-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088305.D
Acq On : 23 Jun 2016 23:09
Operator : UM/SJ
Sample : H3607-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P0-002

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
2-Pentanone, 4-hy...	4.73	2.6	ng	66120	1	6.59	507649	20.0
unknown6.36	6.36	60.1	ng	1525390	1	6.59	507649	20.0
Benzenesulfonamid...	10.50	2.4	ng	91275	4	11.11	768709	20.0
2,4,6-Trichlorobe...	11.71	2.7	ng	105202	4	11.11	768709	20.0
Hexadecanoic acid...	12.51	10.4	ng	331538	5	13.73	639033	20.0
n-Nonadecanol-1	12.59	2.2	ng	70910	5	13.73	639033	20.0
Octadecanoic acid...	13.22	6.2	ng	196908	5	13.73	639033	20.0
Octacosane	13.27	2.1	ng	67664	5	13.73	639033	20.0
Tetratetracontane	13.59	3.3	ng	104783	5	13.73	639033	20.0
Hexacosane	14.21	2.0	ng	64902	5	13.73	639033	20.0
Heneicosane	14.50	2.7	ng	75959	6	15.09	561643	20.0
Eicosane	14.79	2.0	ng	56993	6	15.09	561643	20.0