LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088631.D
Acq On : 2 Jul 2016 22:01
Operator : UM/SJ
Sample : H3837-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.2-7

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-BF063016.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	1.861	22	24	33	rVB	34403	56819	1.98%	0.204%
2	1.998	33	36	40	rVB2	49052	73477	2.56%	0.264%
3	2.993	120	123	130	rBV	21078	44510	1.55%	0.160%
4	4.959	292	295	301	rBV	230441	318811	11.10%	1.145%
5	5.382	329	332	335	rBV	1853540	2396141	83.44%	8.602%
6	6.433	420	424	426	rVB	2368811	2871817	100.00%	10.310%
7	6.559	432	435	438	rBV	2425111	2391206	83.26%	8.584%
8	6.799	453	456	457	rBV	535693	728489	25.37%	2.615%
9	6.947	467	469	471	rVB	1933385	1909317	66.48%	6.854%
10	7.359	502	505	507	rBV	1823415	1747333	60.84%	6.273%
11	8.079	565	568	570	rBV	1257980	1022295	35.60%	3.670%
12	9.153	660	662	665	rBV	2366822	2791294	97.20%	10.021%
13	9.553	695	697	699	rBV	170815	187649	6.53%	0.674%
14	9.691	707	709	711	rBV	74258	63811	2.22%	0.229%
15	9.828	719	721	723	rVB	1145318	981041	34.16%	3.522%
16	10.273	758	760	762	rVB	38398	29583	1.03%	0.106%
17	10.616	787	790	792	rBV	1456895	1490813	51.91%	5.352%
18	10.742	799	801	805	rVB	45594	57616	2.01%	0.207%
19	11.188	838	840	842	rBV	66885	65522	2.28%	0.235%
20	11.302	848	850	853	rBV	744183	808359	28.15%	2.902%
21	11.382	854	857	858	rVB2	78046	82420	2.87%	0.296%
22	11.531	869	870	874	rVV2	35272	39076	1.36%	0.140%
23	11.851	895	898	899	rBV	92150	116095	4.04%	0.417%
24	11.919	902	904	908	rVB2	21123	33314	1.16%	0.120%
25	12.114	918	921	925	rVB	22511	43806	1.53%	0.157%
26	12.514	953	956	958	rBV	391517	365823	12.74%	1.313%
27	12.628	965	966	968	rBV2	34219	37413	1.30%	0.134%
28	12.742	972	976	978	rBV	280682	368944	12.85%	1.325%
29	12.891	987	989	991	rBV	2088724	1934905	67.38%	6.946%
30	12.959	991	995	1001	rBV4	27779	49328	1.72%	0.177%
31	13.051	1001	1003	1006	rBV	30029	74112	2.58%	0.266%
32	13.131	1006	1010	1012	rBV2	41307	75581	2.63%	0.271%
33	13.165	1012	1013	1017	rBV2	36538	62389	2.17%	0.224%
34	13.268	1017	1022	1023	rBV2	26648	55078	1.92%	0.198%

LSC Area Percent Report

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Instrument : BNA_F
ClientSampleId : C1.2-7

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.371	1029	1031	1035	rVB3	21200	39294	1.37%	0.141%
36	13.474	1038	1040	1043	rVB2	36498	41860	1.46%	0.150%
37	13.565	1046	1048	1051	rBV	65445	85452	2.98%	0.307%
38	13.679	1055	1058	1060	rBV	56265	98651	3.44%	0.354%
39	13.714	1060	1061	1062	rBV	37831	36201	1.26%	0.130%
40	13.794	1067	1068	1072	rVB2	165863	226180	7.88%	0.812%
41	13.931	1077	1080	1086	rBV2	850628	1295945	45.13%	4.652%
42	14.354	1115	1117	1119	rVB	62613	57661	2.01%	0.207%
43	14.434	1122	1124	1129	rVB3	66309	174447	6.07%	0.626%
44	14.697	1145	1147	1148	rBV	74456	88046	3.07%	0.316%
45	14.937	1166	1168	1173	rBV	297715	656323	22.85%	2.356%
46	15.040	1175	1177	1178	rVB	91549	96786	3.37%	0.347%
47	15.223	1190	1193	1196	rVB	170563	224300	7.81%	0.805%
48	15.280	1196	1198	1200	rBV	104345	167860	5.85%	0.603%
49	15.337	1200	1203	1209	rVB	485883	703077	24.48%	2.524%
50	15.794	1241	1243	1245	rBV	68508	112653	3.92%	0.404%
51	16.674	1317	1320	1329	rVB2	90093	265919	9.26%	0.955%
52	17.074	1353	1355	1361	rVB	57393	110418	3.84%	0.396%

Sum of corrected areas: 27855260

LSC Report - Integrated Chromatogram

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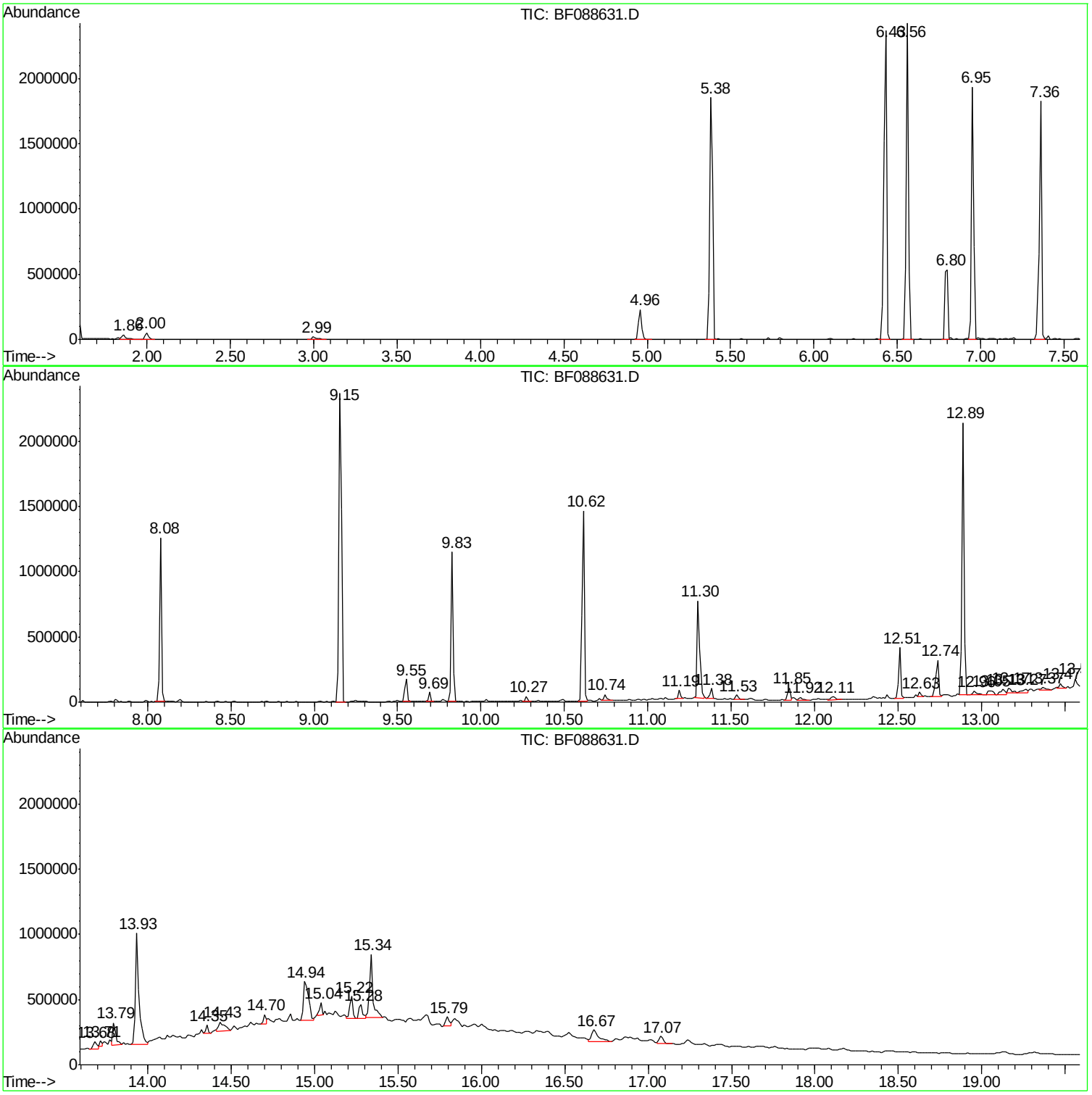
Sample : H3837-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.2-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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\BF070216\
Data File : BF088631.D
Acq On : 2 Jul 2016 22:01
Operator : UM/SJ
Sample : H3837-05
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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.2-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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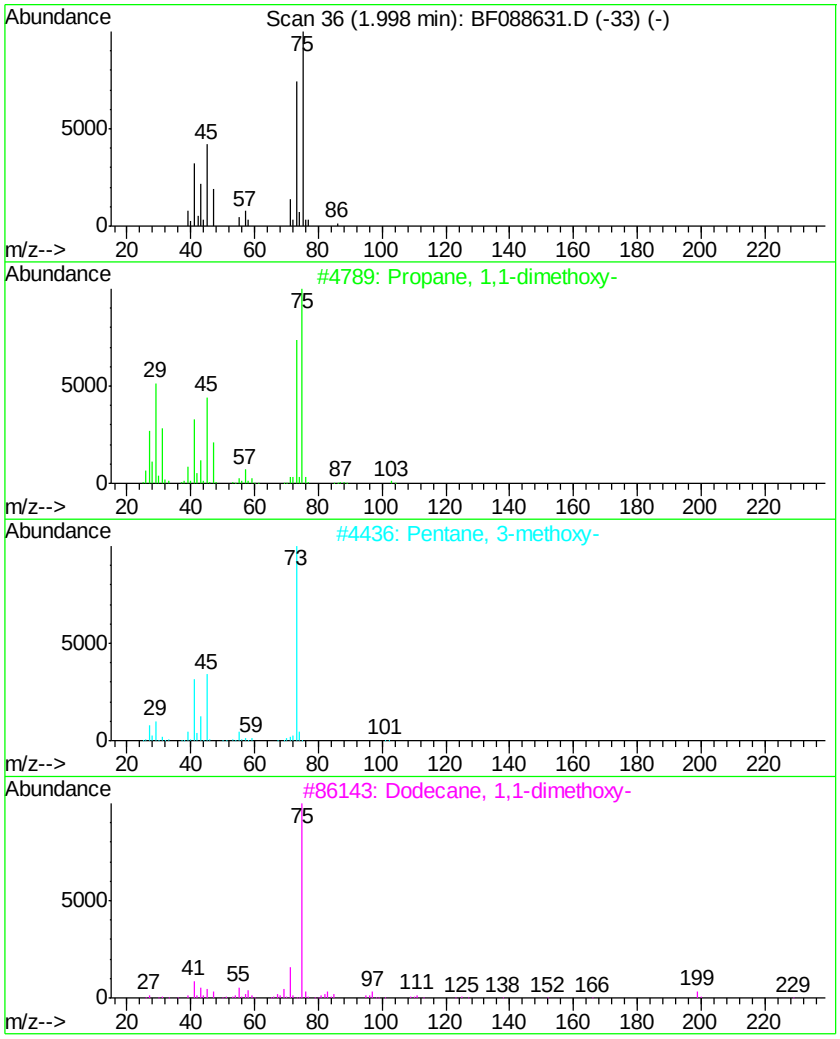
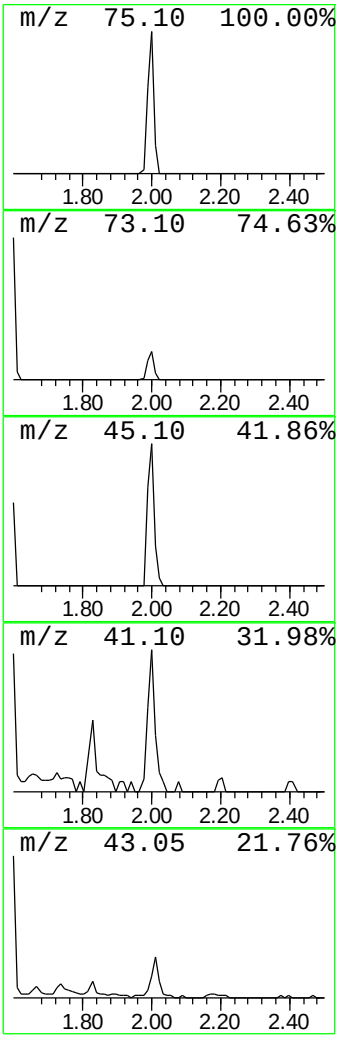
Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	2.02 ng	73477	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	Dodecane, 1,1-dimethoxy-	230	C14H30O2	014620-52-1	9
4	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
5	Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	9





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.2-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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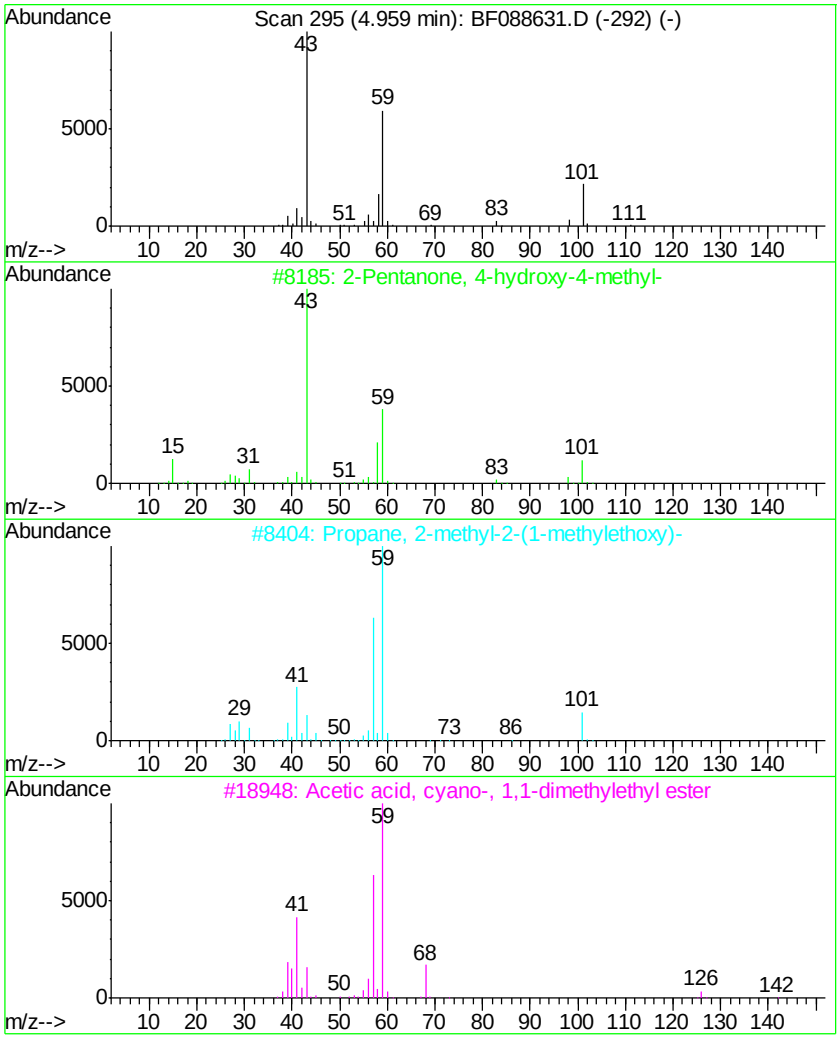
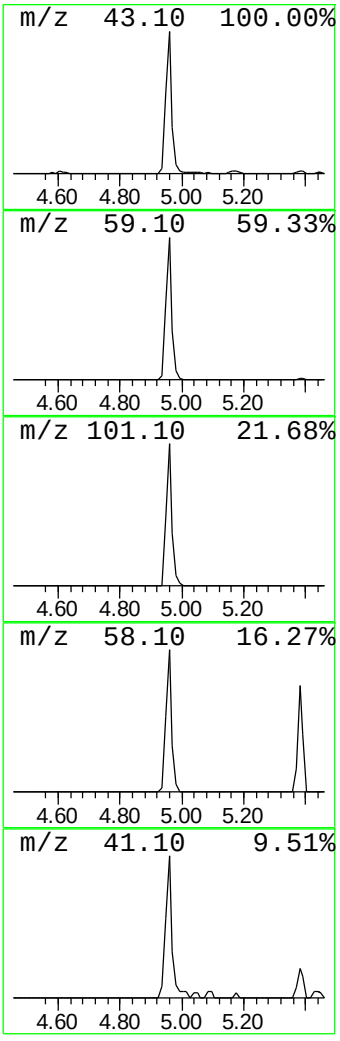
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	8.75 ng	318811	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF088631.D
Acq On : 2 Jul 2016 22:01
Operator : UM/SJ
Sample : H3837-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.2-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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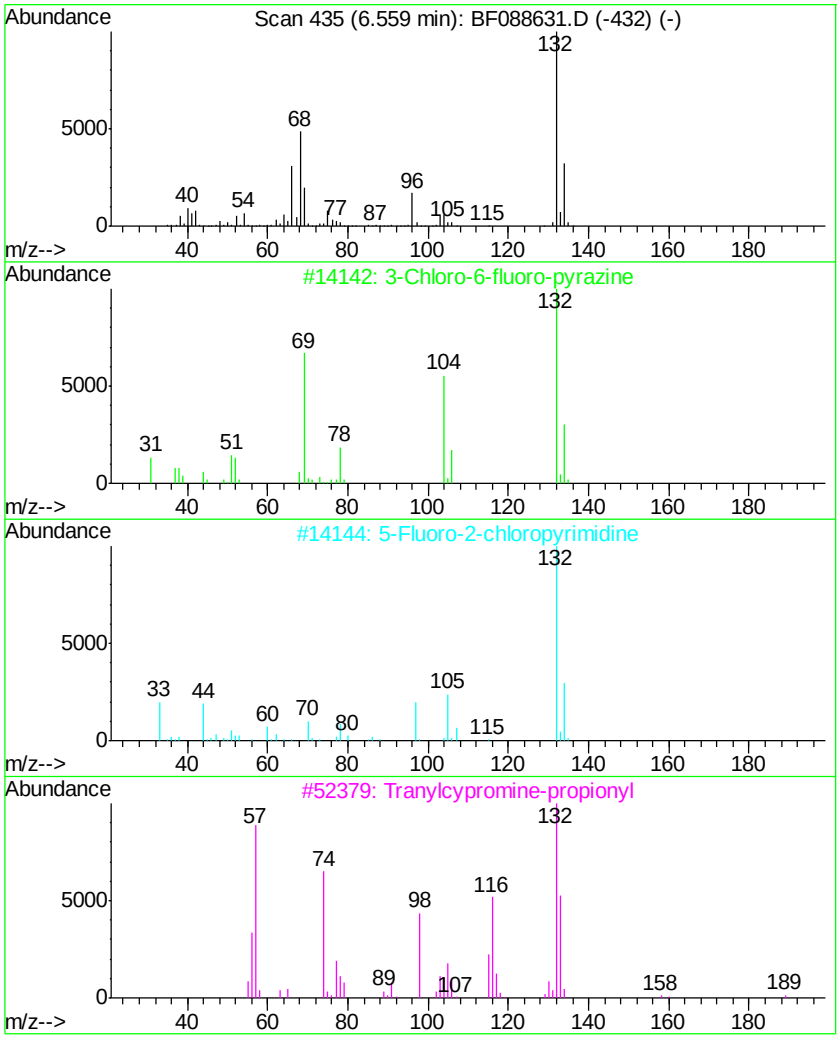
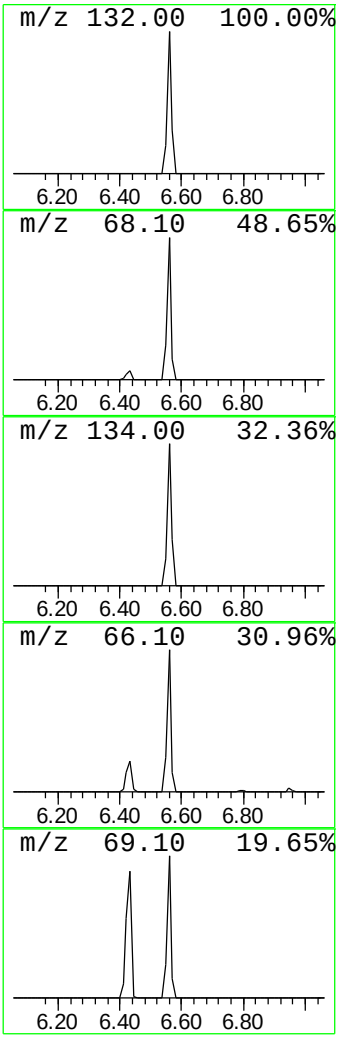
Peak Number 3 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	65.65 ng	2391210	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Sample : H3837-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.2-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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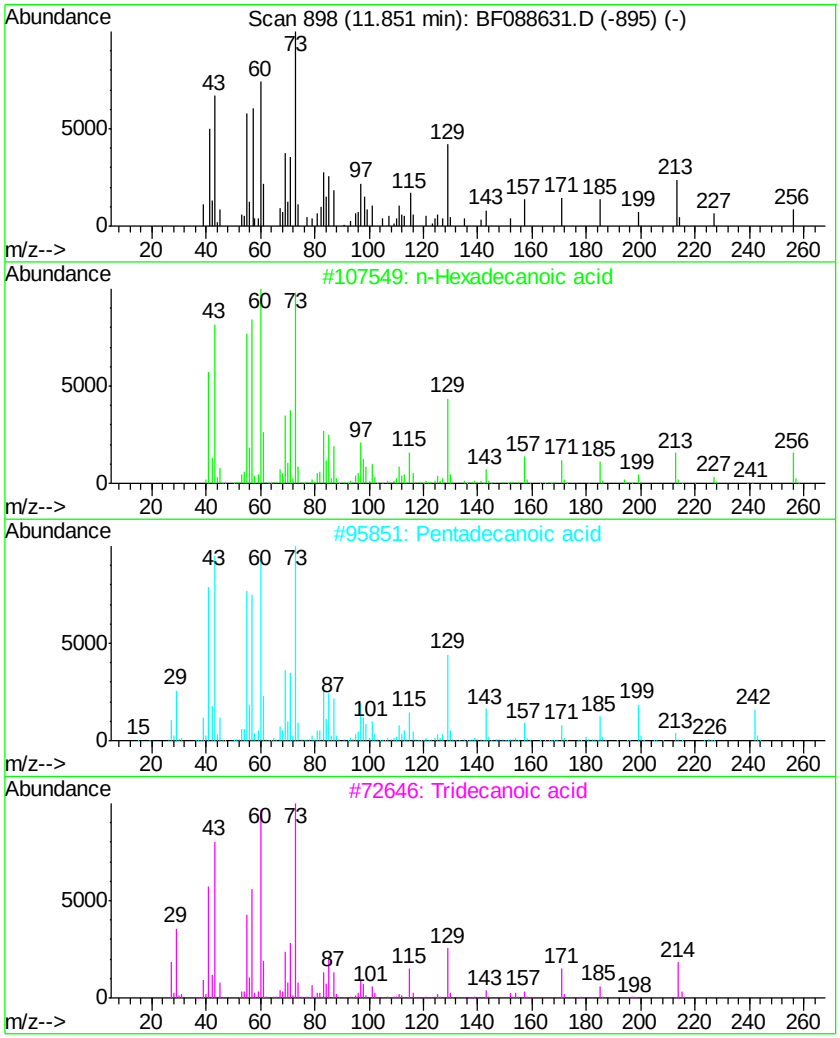
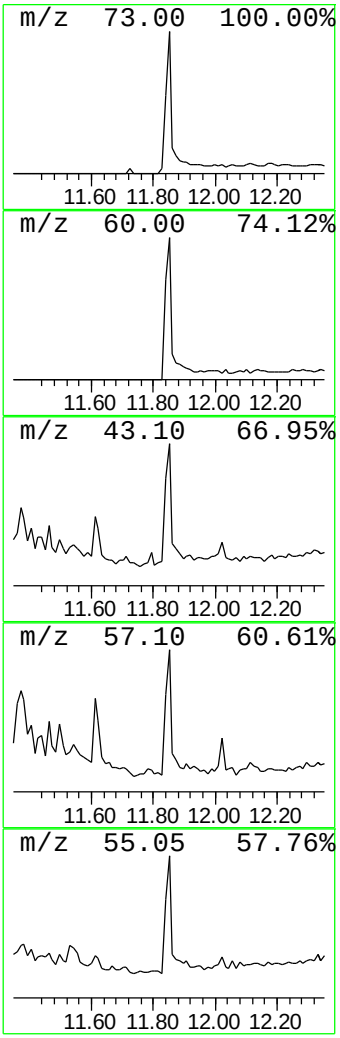
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.87 ng	116095	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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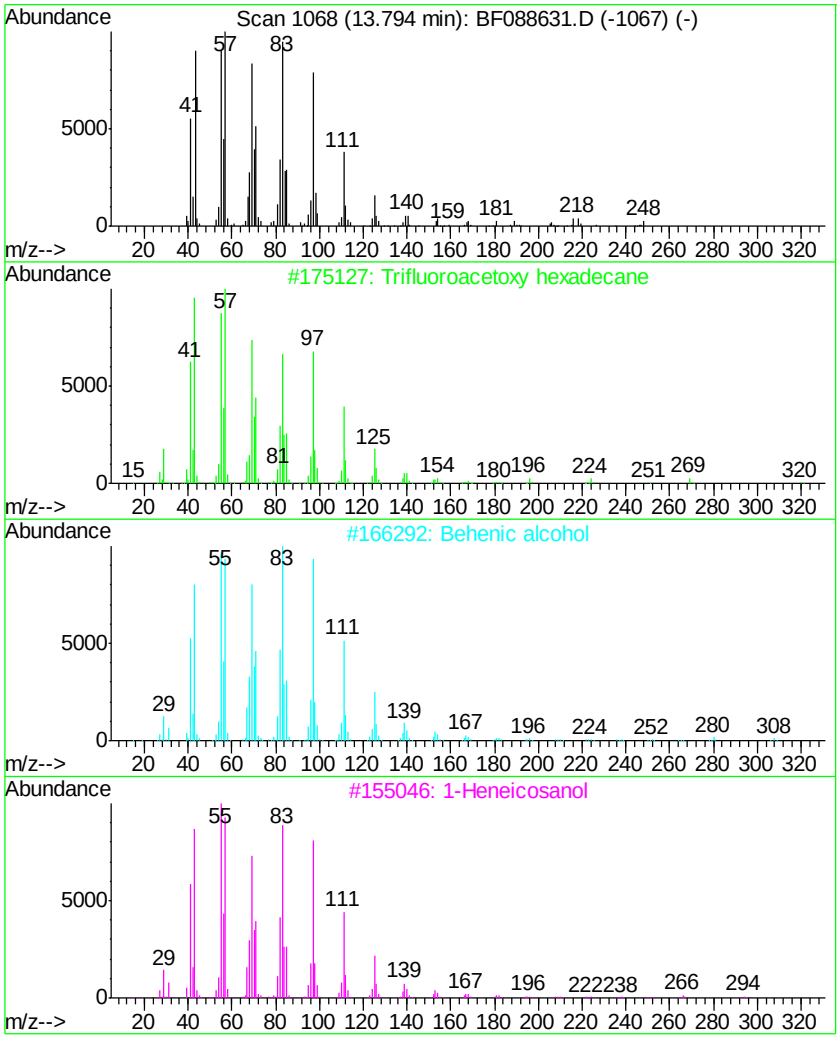
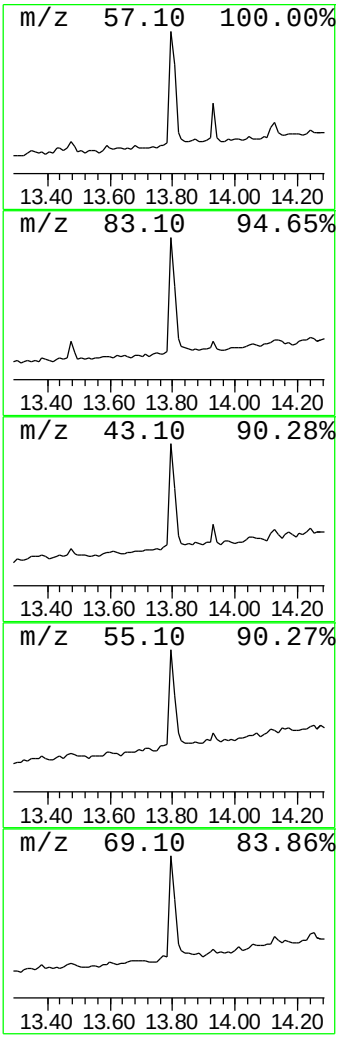
Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.49 ng	226180	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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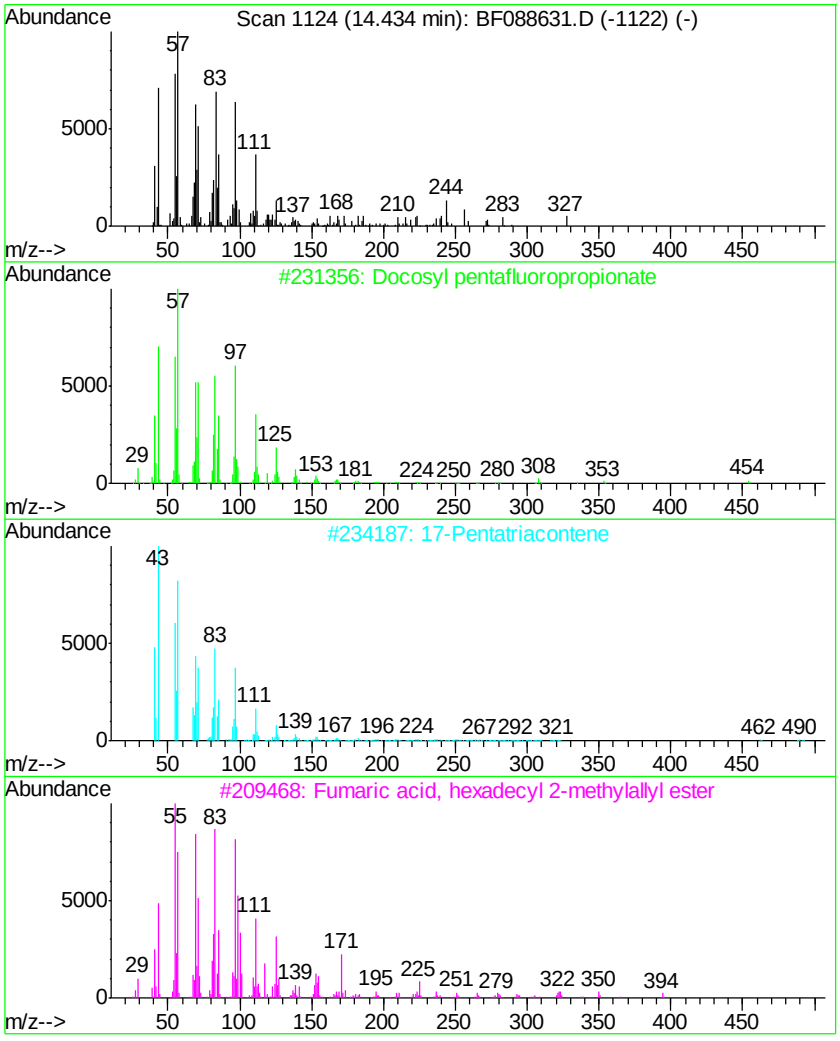
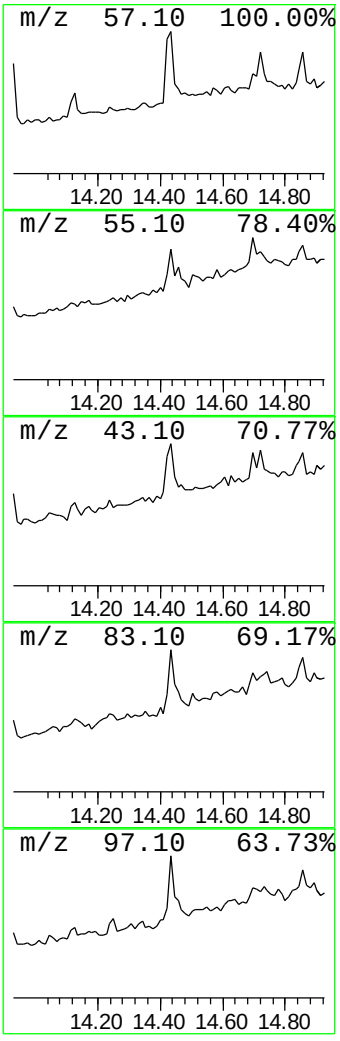
Peak Number 8 Docosyl pentafluoropropionate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.69 ng	174447	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	83
2	17-Pentatriacontene	491	C35H70	006971-40-0	83
3	Fumaric acid, hexadecyl 2-methyl...	394	C24H42O4	1000330-55-5	74
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	68
5	1-Heneicosanol	312	C21H44O	015594-90-8	62





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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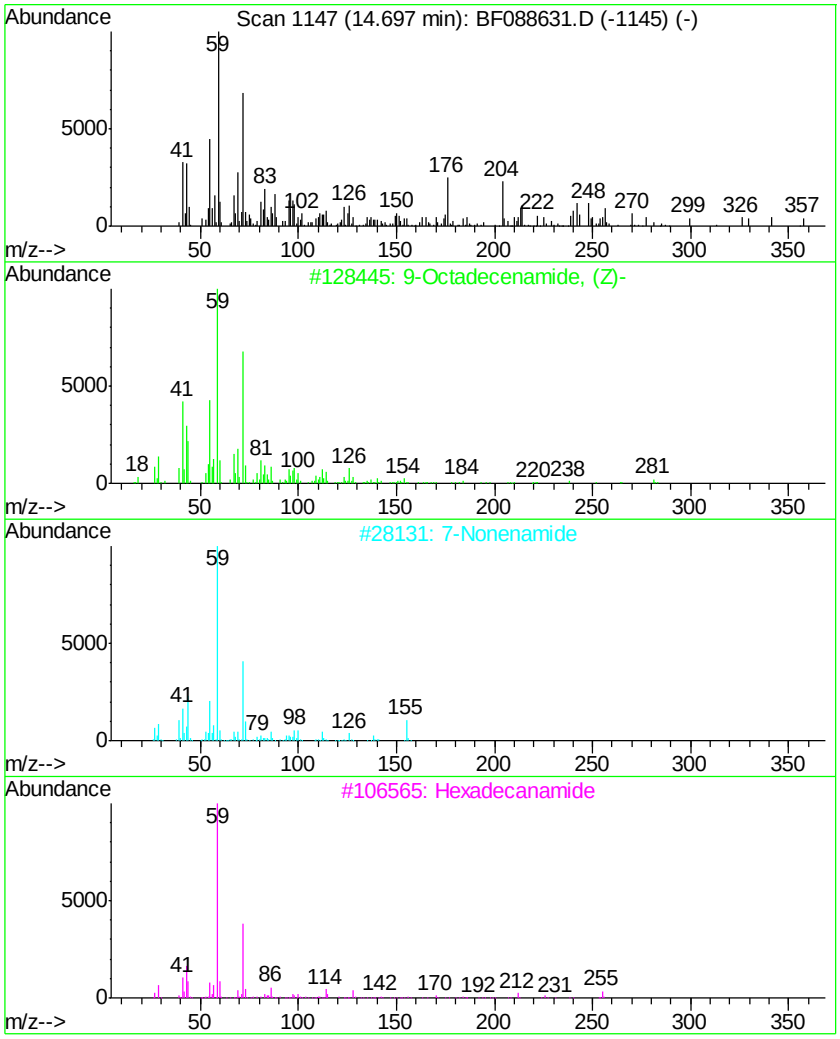
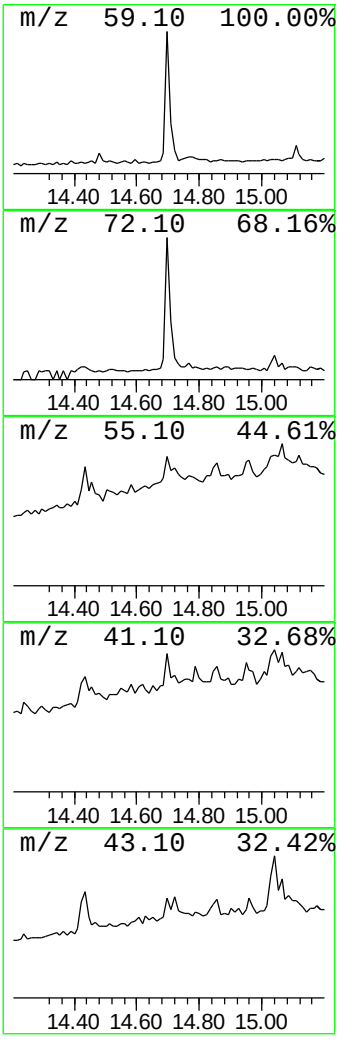
Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	2.50 ng	88046	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	7-Nonenamide	155	C9H17NO	090949-53-4	49
3	Hexadecanamide	255	C16H33NO	000629-54-9	49
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	47
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	42





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Sample : H3837-05
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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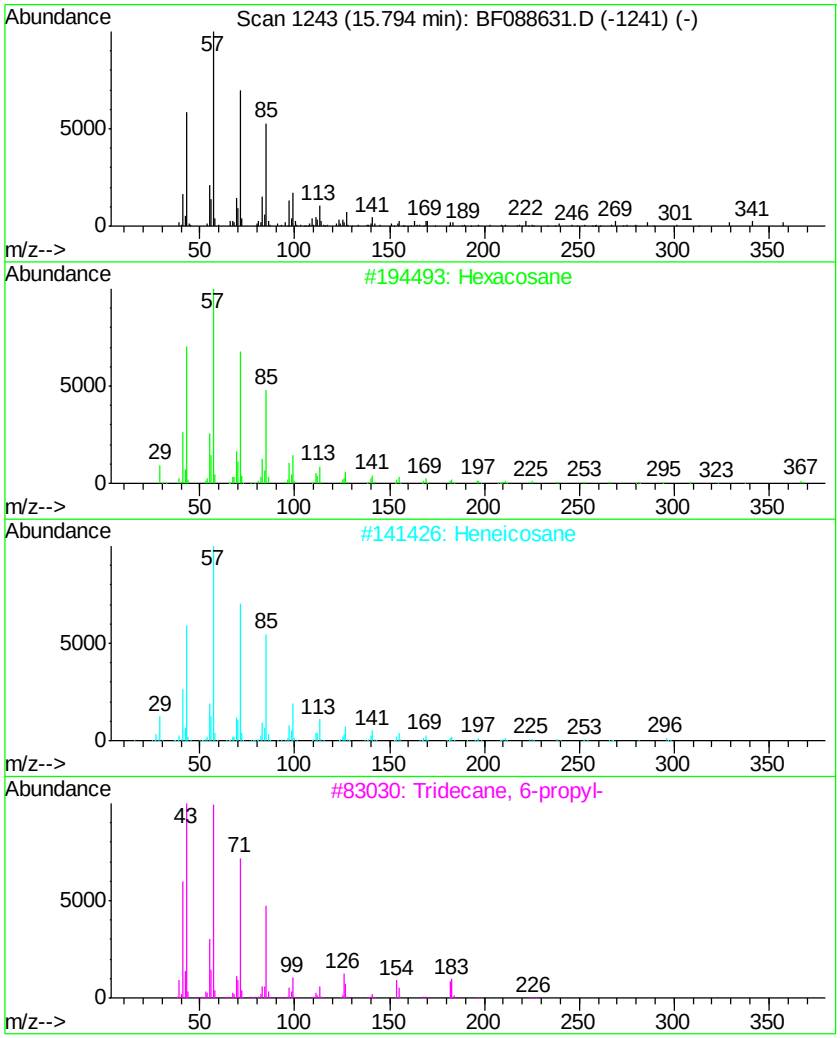
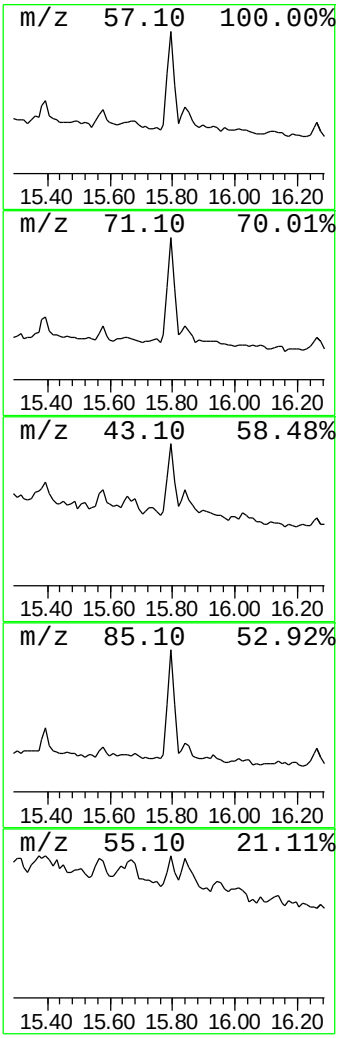
Peak Number 12 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	3.20 ng	112653	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heneicosane	296	C21H44	000629-94-7	87
3	Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Octadecane	254	C18H38	000593-45-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088631.D
Acq On : 2 Jul 2016 22:01
Operator : UM/SJ
Sample : H3837-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C1.2-7

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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...	2.00	2.0	ng	73477	1	6.80	728489	20.0
2-Pentanone, 4-hy...	4.96	8.8	ng	318811	1	6.80	728489	20.0
unknown6.56	6.56	65.7	ng	2391210	1	6.80	728489	20.0
n-Hexadecanoic acid	11.85	2.9	ng	116095	4	11.30	808359	20.0
Trifluoroacetoxy ...	13.79	3.5	ng	226180	5	13.93	1295950	20.0
Docosyl pentafluo...	14.43	2.7	ng	174447	5	13.93	1295950	20.0
9-Octadecenamide,...	14.70	2.5	ng	88046	6	15.34	703077	20.0
Hexacosane	15.79	3.2	ng	112653	6	15.34	703077	20.0