LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088048.D
Acq On : 15 Jun 2016 22:05
Operator : UM/SJ
Sample : H3474-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-B3(7-15)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	1.690	8	9	18	rVV	287181	543070	20.12%	2.276%
2	1.815	18	20	32	rVV	1556933	2699604	100.00%	11.312%
3	1.964	32	33	50	rVB	79121	258780	9.59%	1.084%
4	4.913	288	291	306	rBV	142013	201330	7.46%	0.844%
5	5.336	325	328	331	rBV	1792587	1849485	68.51%	7.749%
6	5.976	383	384	388	rBV2	37197	63031	2.33%	0.264%
7	6.044	388	390	391	rBV	22633	33738	1.25%	0.141%
8	6.170	398	401	405	rBV	23932	46579	1.73%	0.195%
9	6.262	408	409	411	rBV2	35488	36436	1.35%	0.153%
10	6.387	417	420	422	rBV	1808531	1948691	72.18%	8.165%
11	6.479	426	428	429	rBV	43744	67692	2.51%	0.284%
12	6.513	429	431	433	rVB	2040557	2139305	79.25%	8.964%
13	6.684	442	446	449	rBV3	17020	51988	1.93%	0.218%
14	6.742	449	451	452	rVV	787087	655840	24.29%	2.748%
15	6.799	455	456	458	rBV	28688	37568	1.39%	0.157%
16	6.902	463	465	467	rVV	1797051	1821003	67.45%	7.630%
17	6.982	469	472	473	rBV3	17095	31455	1.17%	0.132%
18	7.027	473	476	478	rVB3	29568	47496	1.76%	0.199%
19	7.142	484	486	487	rBV	51314	60216	2.23%	0.252%
20	7.313	498	501	503	rVB	1362802	1470486	54.47%	6.161%
21	7.393	506	508	510	rVB2	32583	46117	1.71%	0.193%
22	7.519	516	519	520	rBV3	25501	33452	1.24%	0.140%
23	7.553	520	522	523	rVB2	36576	41186	1.53%	0.173%
24	7.667	528	532	535	rBV4	33991	68854	2.55%	0.289%
25	7.770	539	541	546	rVB	60724	65198	2.42%	0.273%
26	8.033	561	564	566	rBV	670726	826755	30.63%	3.464%
27	9.108	655	658	660	rBV	2311767	2103640	77.92%	8.814%
28	9.508	690	693	695	rBV	276387	284254	10.53%	1.191%
29	9.725	710	712	714	rVV	54878	45137	1.67%	0.189%
30	9.782	714	717	719	rVB	998521	882212	32.68%	3.697%
31	10.216	754	755	757	rVB	47610	52678	1.95%	0.221%
32	10.445	771	775	778	rBV	22069	41348	1.53%	0.173%
33	10.571	783	786	788	rBV	1060255	1155563	42.80%	4.842%
34	10.696	795	797	801	rBV	61360	89693	3.32%	0.376%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088048.D
Acq On : 15 Jun 2016 22:05
Operator : UM/SJ
Sample : H3474-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-B3(7-15)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	11.142	834	836	837	rBV	31682	30690	1.14%	0.129%
36	11.256	844	846	849	rBV	722480	698421	25.87%	2.926%
37	12.514	954	956	958	rVB	36704	31557	1.17%	0.132%
38	12.674	968	970	973	rBV2	69257	84209	3.12%	0.353%
39	12.845	982	985	987	rBV	1734252	1574441	58.32%	6.597%
40	13.382	1029	1032	1034	rBV	42628	41733	1.55%	0.175%
41	13.748	1062	1064	1070	rBV	36047	73336	2.72%	0.307%
42	13.897	1074	1077	1079	rBV	478383	670992	24.86%	2.812%
43	14.377	1116	1119	1121	rBV2	22647	36950	1.37%	0.155%
44	14.902	1162	1165	1170	rBV	19331	43785	1.62%	0.183%
45	14.982	1170	1172	1175	rVV2	17114	27695	1.03%	0.116%
46	15.234	1192	1194	1196	rVB	23275	28865	1.07%	0.121%
47	15.291	1196	1199	1205	rVB	537320	665881	24.67%	2.790%
48	15.920	1252	1254	1261	rVB4	13923	29918	1.11%	0.125%
49	16.754	1324	1327	1331	rBV4	10468	27592	1.02%	0.116%

Sum of corrected areas: 23865945

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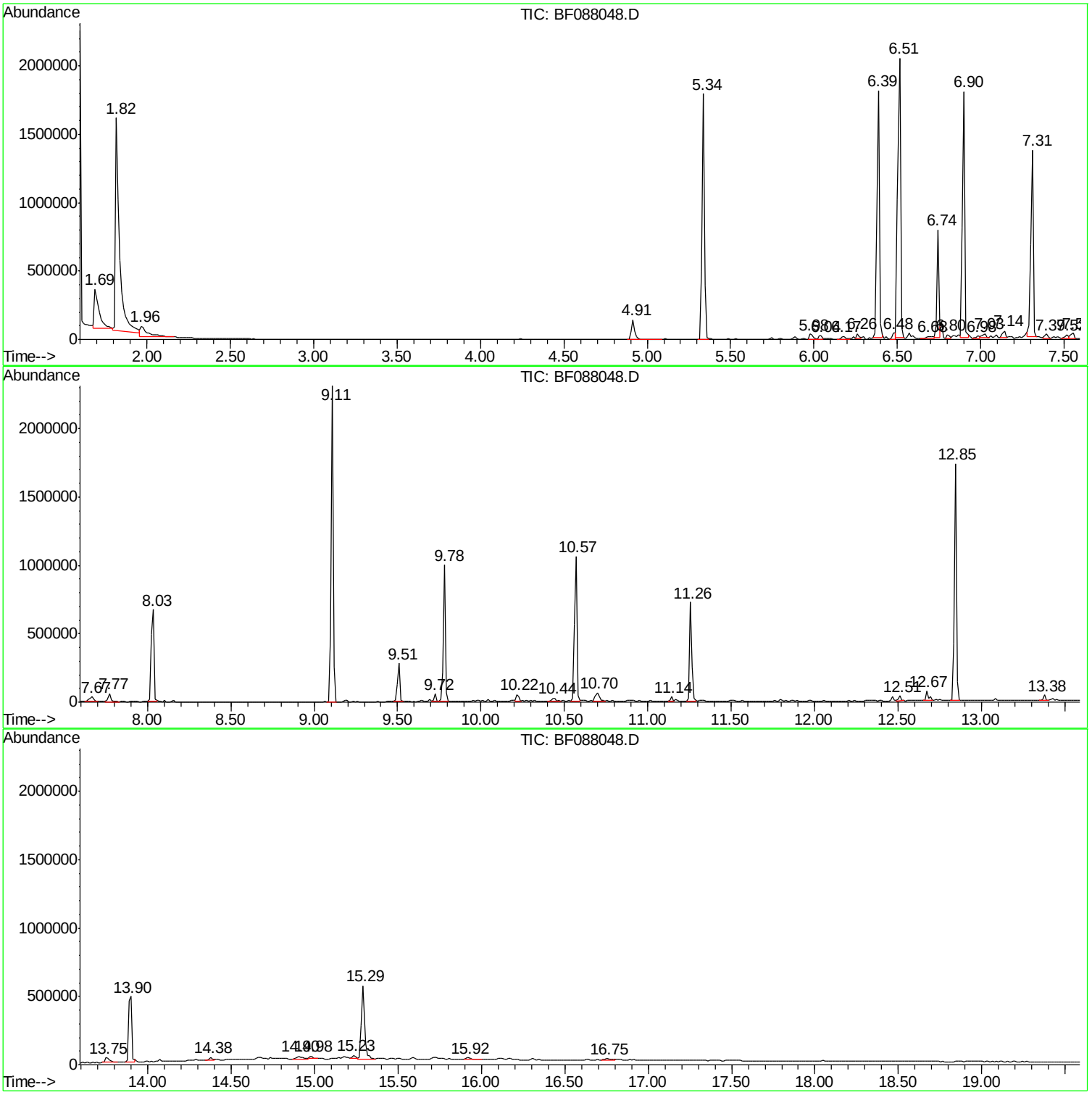
Instrument : BNA_F
ClientSampleId : S6-B3(7-15)C

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\BF061516\
Data File : BF088048.D
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Operator : UM/SJ
Sample : H3474-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-B3(7-15)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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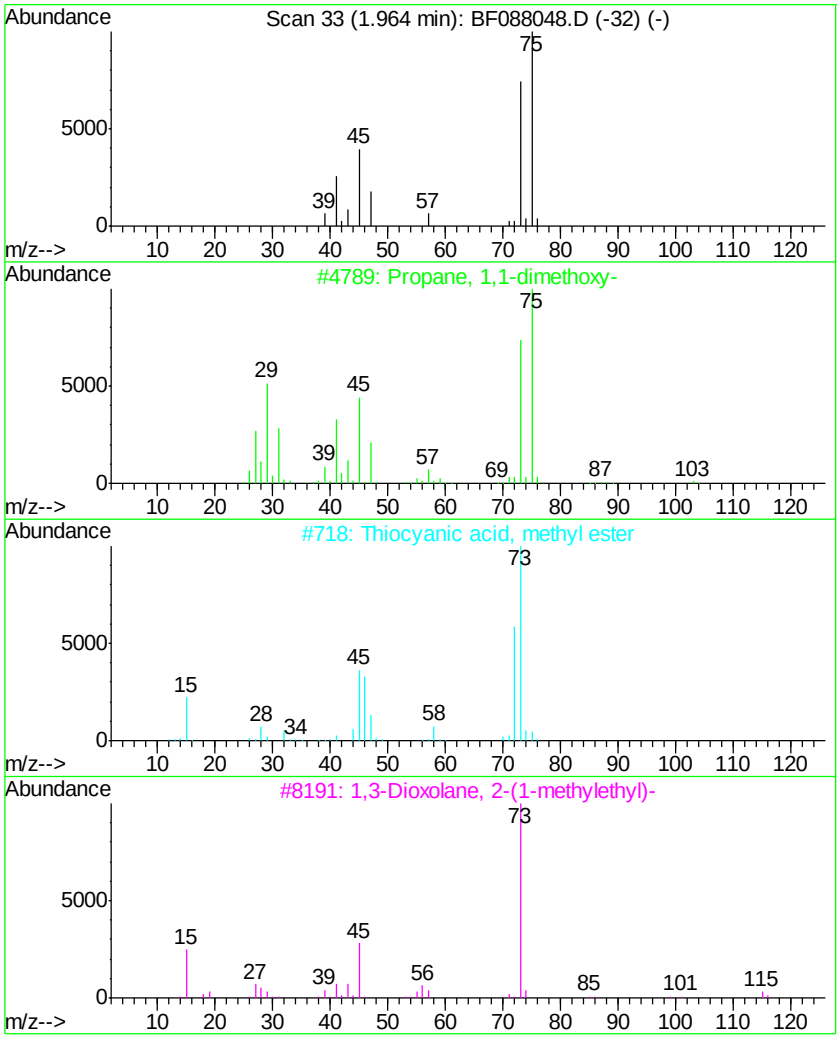
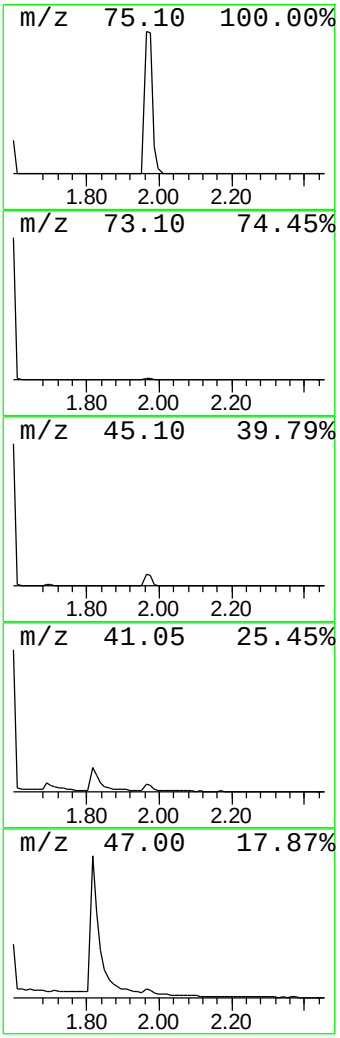
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.96	7.89 ng	258780	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
5	Glycine	75	C2H5NO2	000056-40-6	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088048.D
Acq On : 15 Jun 2016 22:05
Operator : UM/SJ
Sample : H3474-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-B3(7-15)C

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

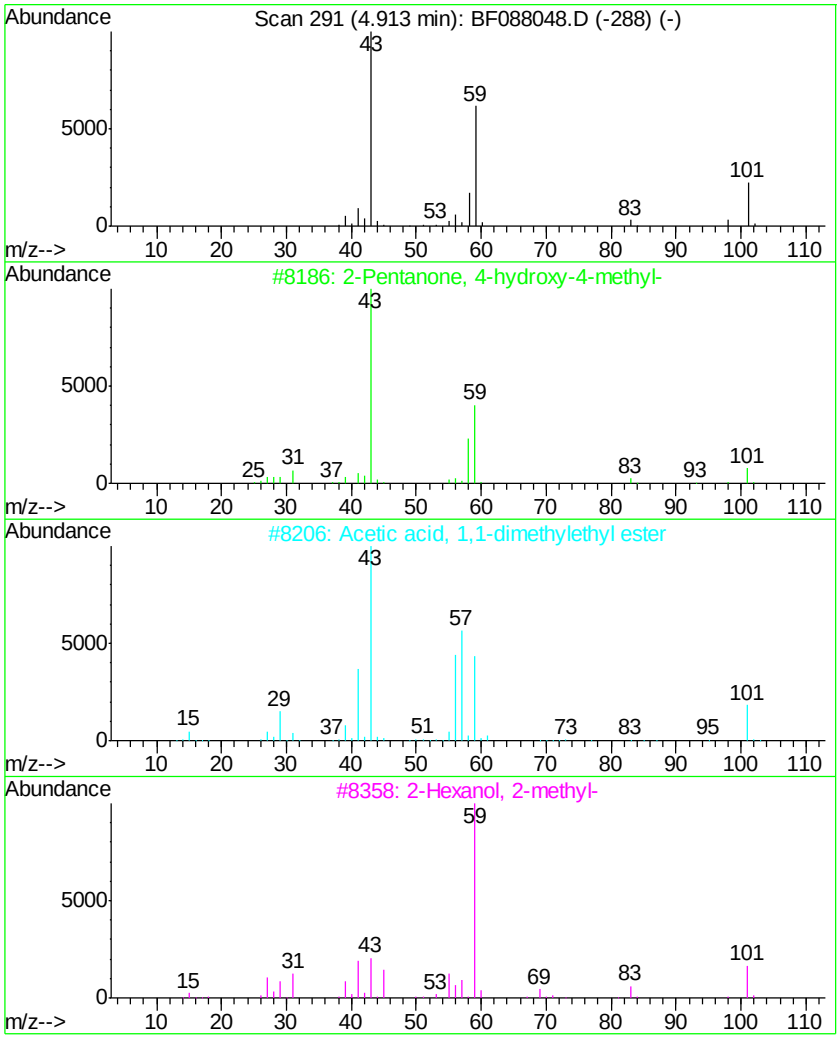
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

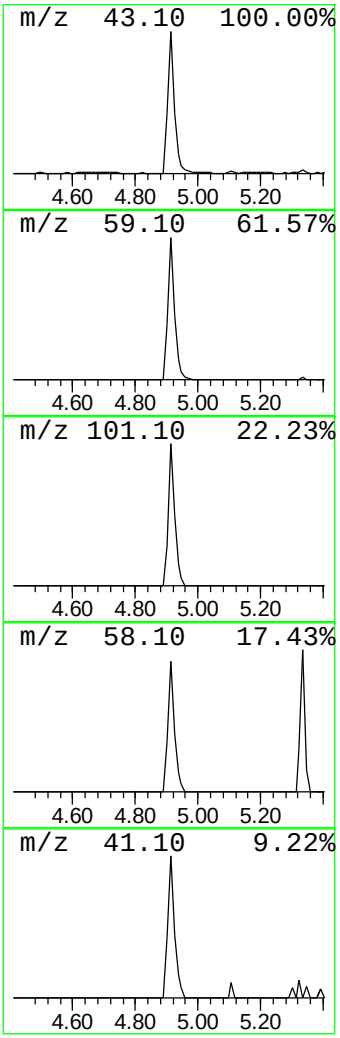
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	6.14 ng	201330	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
Data File : BF088048.D
Acq On : 15 Jun 2016 22:05
Operator : UM/SJ
Sample : H3474-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-B3(7-15)C

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

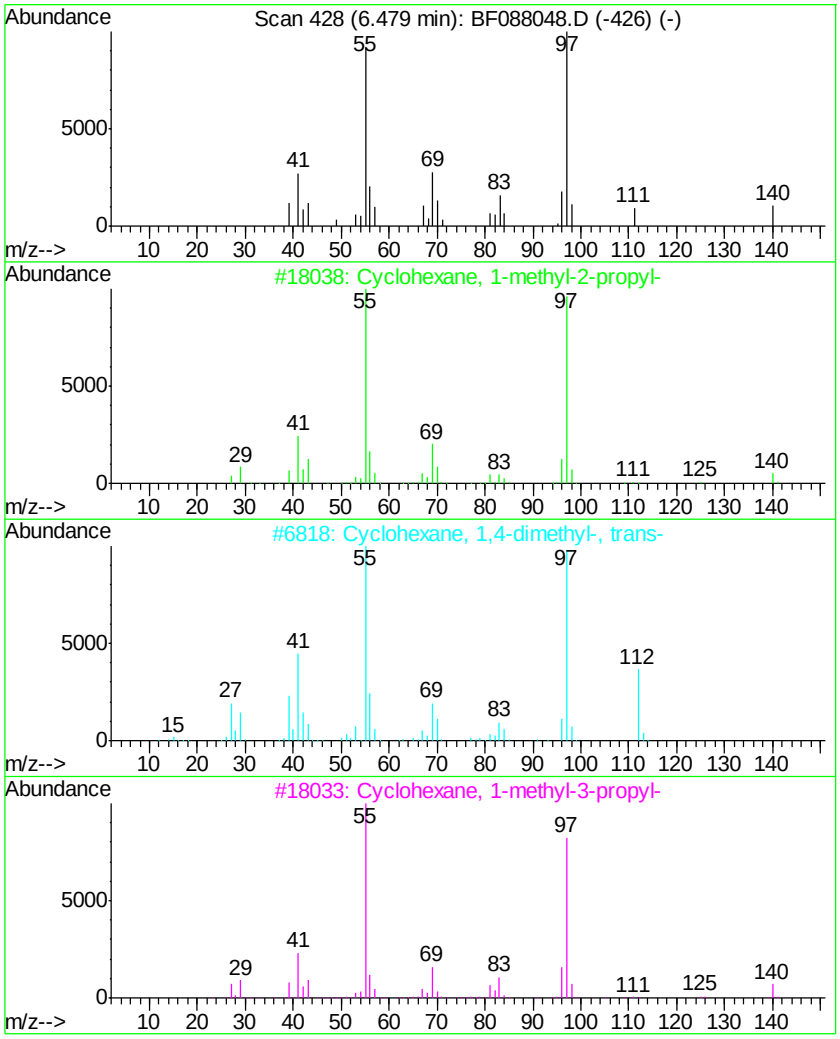
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

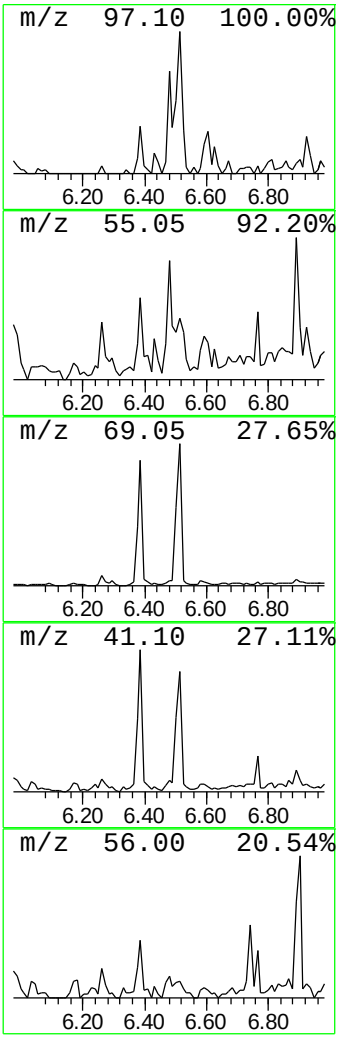
****

Peak Number 5 Cyclohexane, 1-methyl-2-pro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	2.06 ng	67692	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-2-propyl-	140	C10H20	004291-79-6	90
2	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	78
3	Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	72
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	72
5	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061516\
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Sample : H3474-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-B3(7-15)C

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

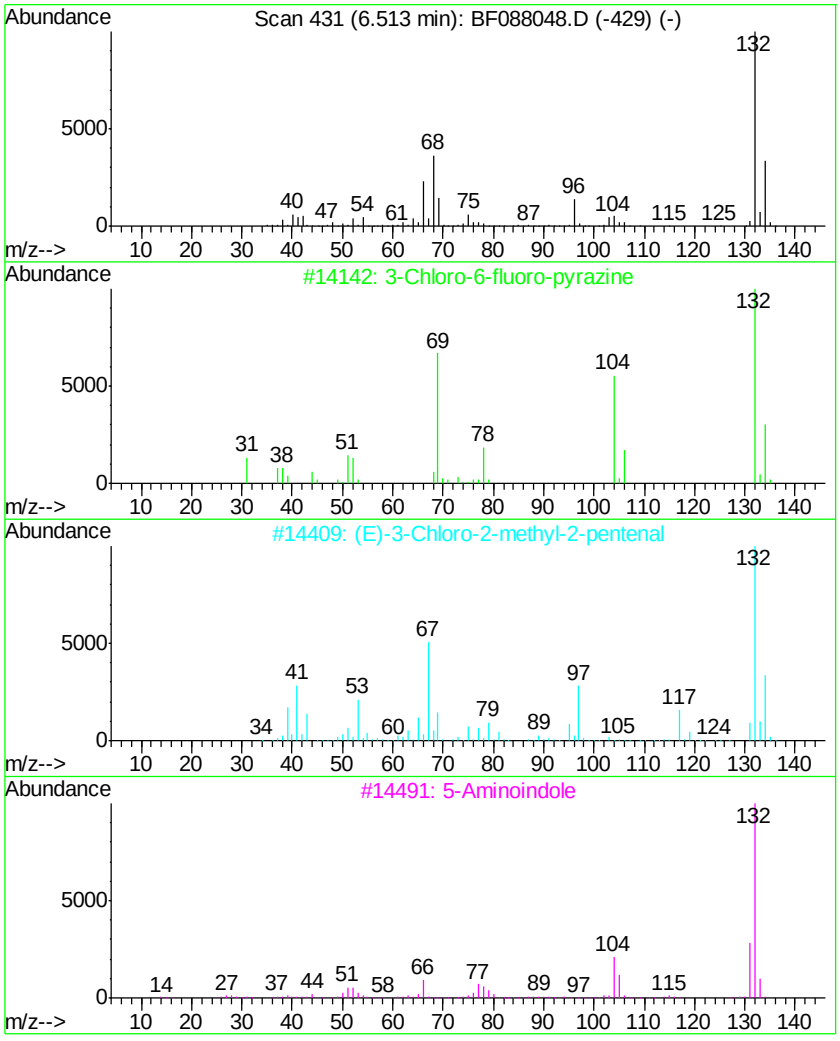
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

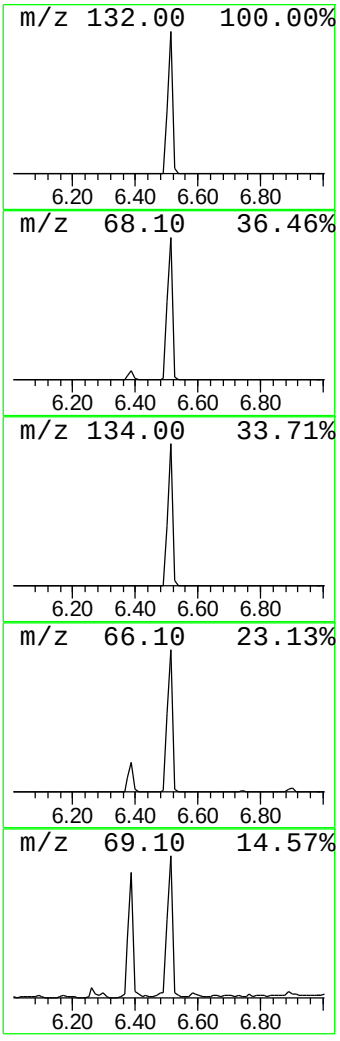
****

Peak Number 6 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	65.24 ng	2139310	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : UM/SJ
Sample : H3474-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-B3(7-15)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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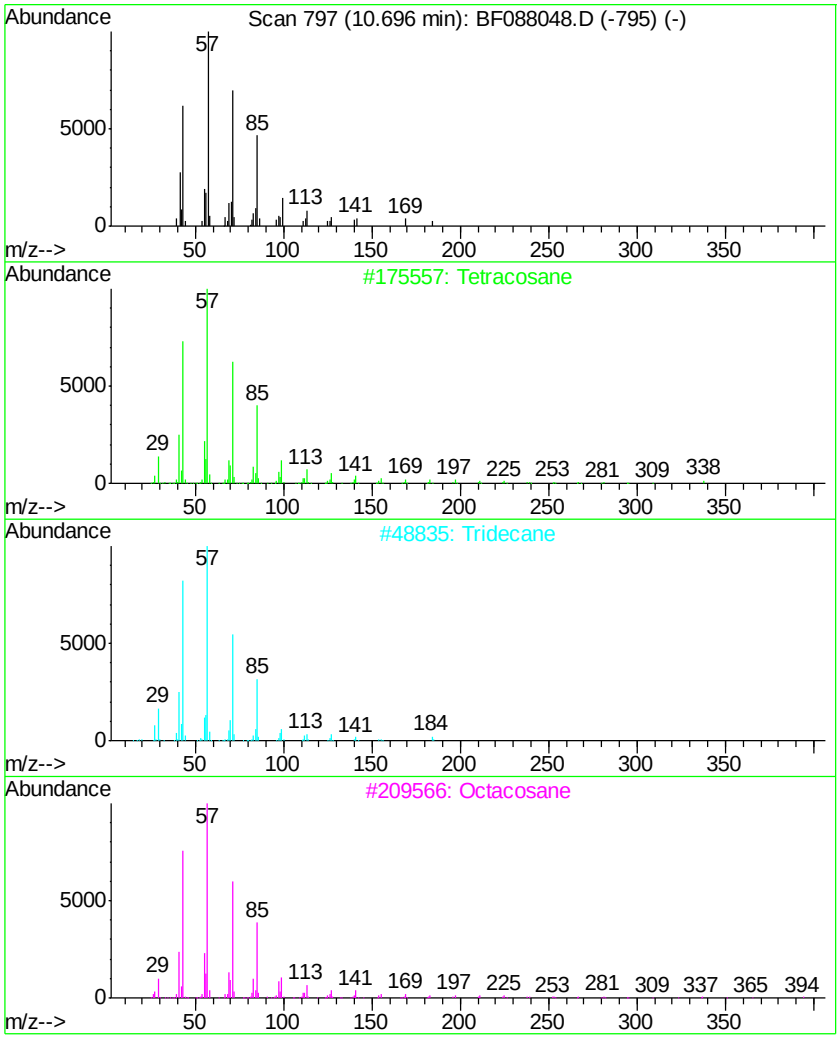
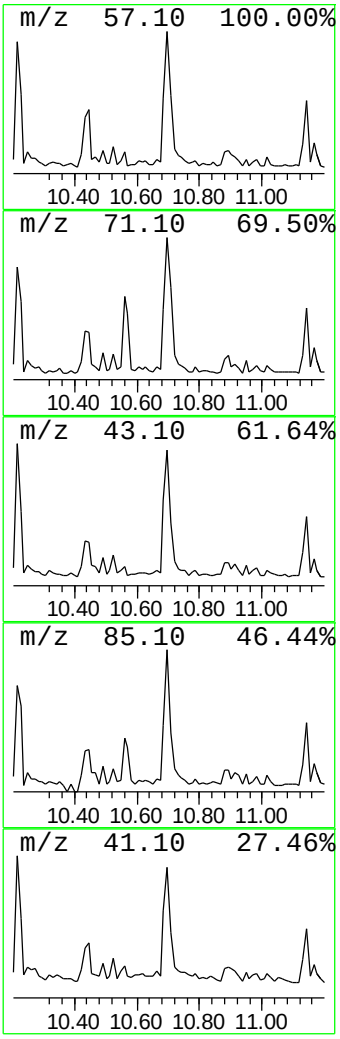
****

Peak Number 8 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.57 ng	89693	Phenanthrene-d10	11.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Tridecane	184	C13H28	000629-50-5	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Hexadecane	226	C16H34	000544-76-3	90





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Sample : H3474-07
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Instrument : BNA_F
ClientSampleId : S6-B3(7-15)C

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

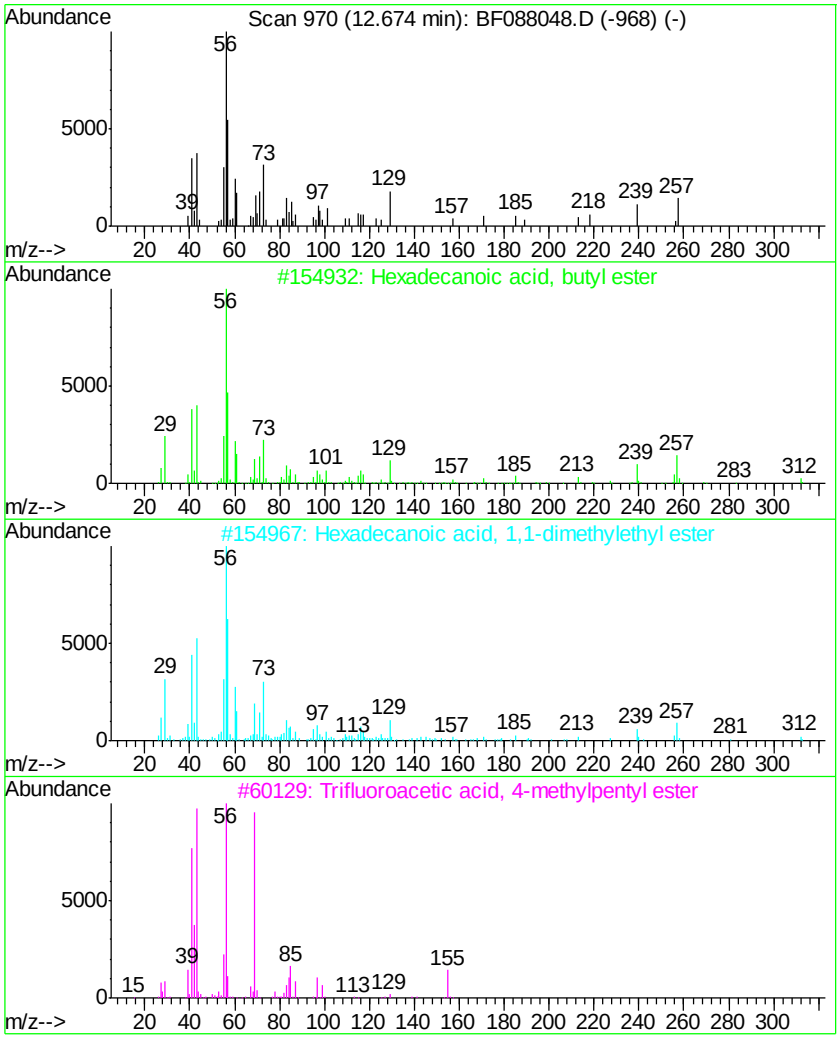
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

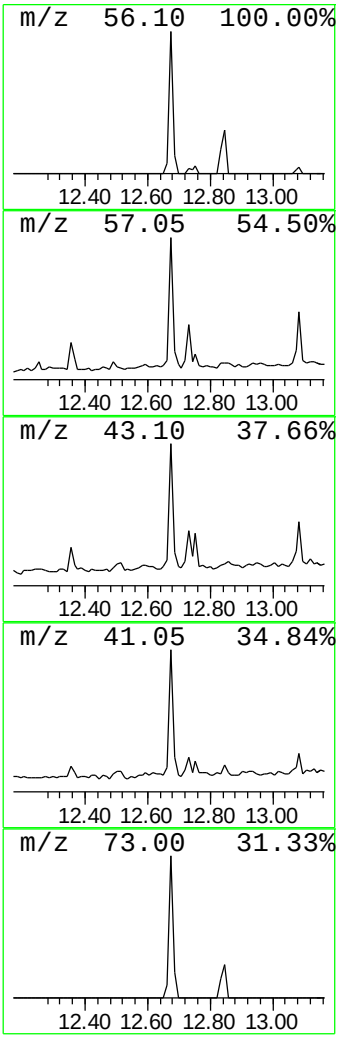
****

Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	2.51 ng	84209	Chrysene-d12	13.90

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	86
3	Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	43
4	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37





Library Search Compound Report

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Operator : UM/SJ
Sample : H3474-07
Misc :
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Instrument : BNA_F
ClientSampleId : S6-B3(7-15)C

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

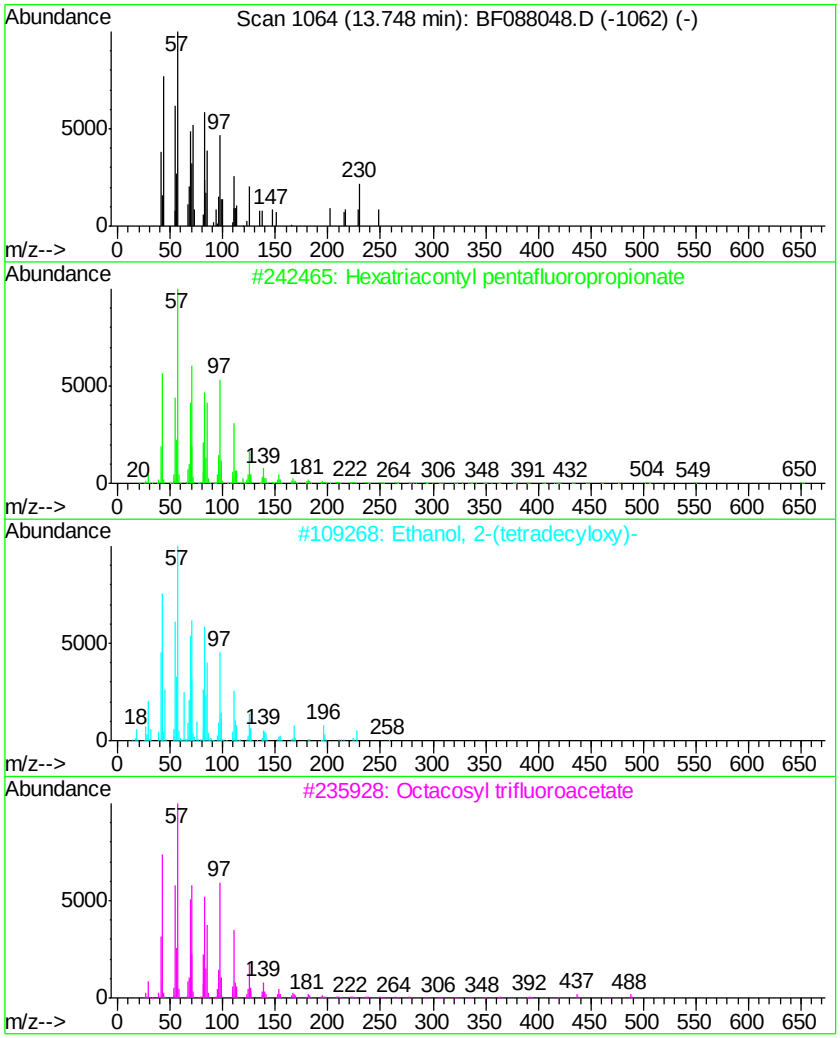
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

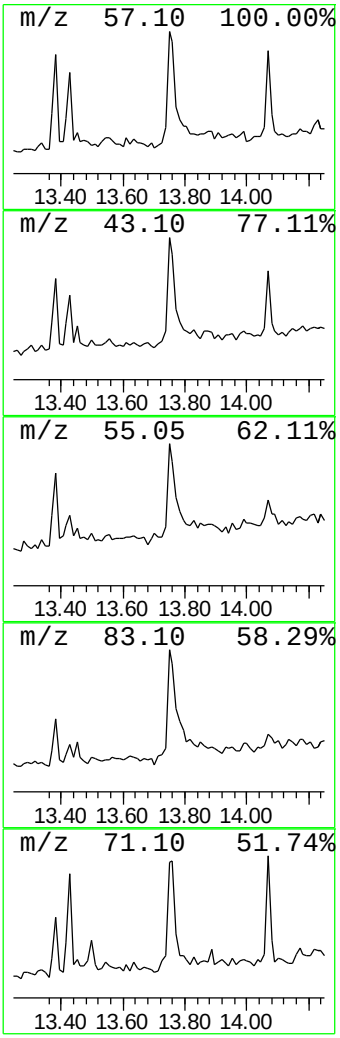
****

Peak Number 10 Hexatriacontyl pentafluorop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	2.19 ng	73336	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	83
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	68
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	62
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	55





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061516\
Data File : BF088048.D
Acq On : 15 Jun 2016 22:05
Operator : UM/SJ
Sample : H3474-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S6-B3(7-15)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...	1.96	7.9	ng	258780	1	6.74	655840	20.0
2-Pentanone, 4-hy...	4.91	6.1	ng	201330	1	6.74	655840	20.0
Cyclohexane, 1-me...	6.48	2.1	ng	67692	1	6.74	655840	20.0
unknown6.51	6.51	65.2	ng	2139310	1	6.74	655840	20.0
Tetracosane	10.70	2.6	ng	89693	4	11.26	698421	20.0
Hexadecanoic acid...	12.67	2.5	ng	84209	5	13.90	670992	20.0
Hexatriacontyl pe...	13.75	2.2	ng	73336	5	13.90	670992	20.0