LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098847.D
Acq On : 26 Sep 2017 22:12
Operator : SJ/JU
Sample : I5427-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-D-S

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-BF092317.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	2.210	16	21	27	rVB	290618	357214	7.33%	1.229%
2	5.134	515	518	528	rVB	268563	276747	5.68%	0.952%
3	5.528	581	585	588	rBV	1738351	1475805	30.28%	5.079%
4	6.528	751	755	758	rBV	1259488	985277	20.22%	3.391%
5	6.681	776	781	784	rBV	2941117	2598463	53.32%	8.942%
6	6.910	817	820	824	rBV	1003570	883962	18.14%	3.042%
7	7.069	843	847	851	rBV	3285044	3357756	68.90%	11.555%
8	7.481	910	917	919	rBV	2507665	2794511	57.34%	9.617%
9	8.192	1034	1038	1042	rBV	1304285	1189708	24.41%	4.094%
10	9.275	1216	1222	1225	rBV	4708215	4873554	100.00%	16.771%
11	9.657	1284	1287	1290	rBV	91072	65891	1.35%	0.227%
12	9.951	1333	1337	1341	rVB	1477532	1252950	25.71%	4.312%
13	10.739	1466	1471	1474	rBV	1916616	1721585	35.33%	5.924%
14	11.439	1586	1590	1593	rBV	1293731	1118688	22.95%	3.850%
15	13.022	1854	1859	1863	rBV	3441910	3654983	75.00%	12.578%
16	13.904	2005	2009	2015	rBV	88082	85898	1.76%	0.296%
17	14.074	2034	2038	2042	rVB	959805	813999	16.70%	2.801%
18	15.563	2286	2291	2304	rVB	610465	866833	17.79%	2.983%
19	16.027	2365	2370	2375	rBV2	76886	117135	2.40%	0.403%
20	16.545	2452	2458	2468	rBV	89719	167985	3.45%	0.578%
21	17.157	2556	2562	2572	rVB2	70131	144922	2.97%	0.499%
22	17.880	2679	2685	2698	rVB2	61487	149241	3.06%	0.514%
23	18.739	2825	2831	2842	rVB3	36915	105935	2.17%	0.365%

Sum of corrected areas: 29059042

LSC Report - Integrated Chromatogram

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Misc :
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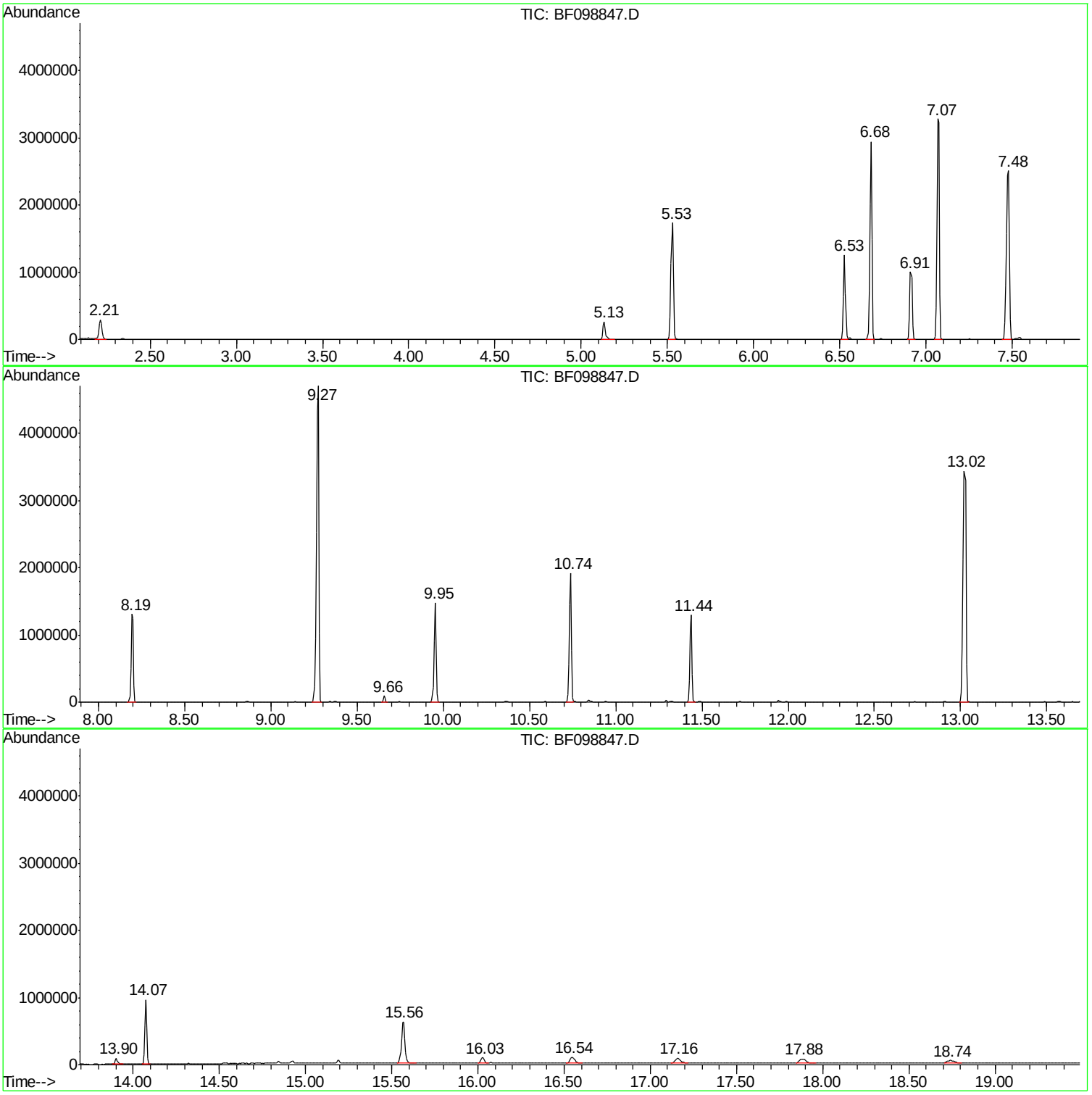
Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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Data File : BF098847.D
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Sample : I5427-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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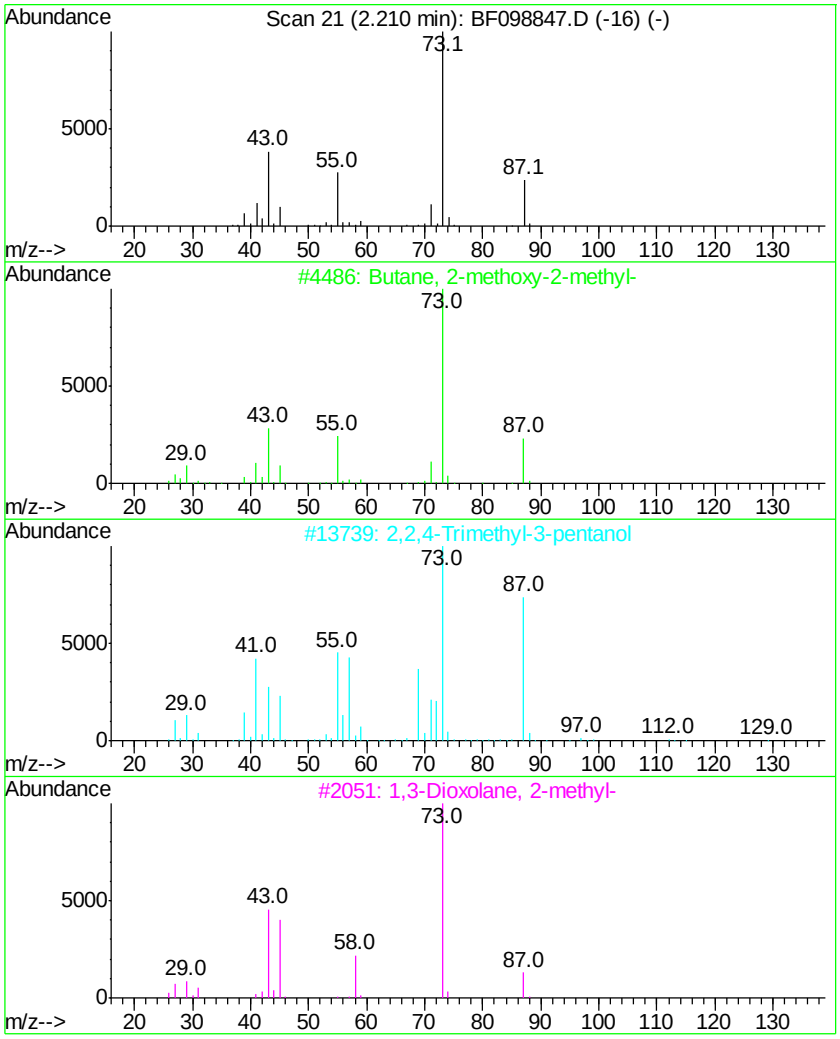
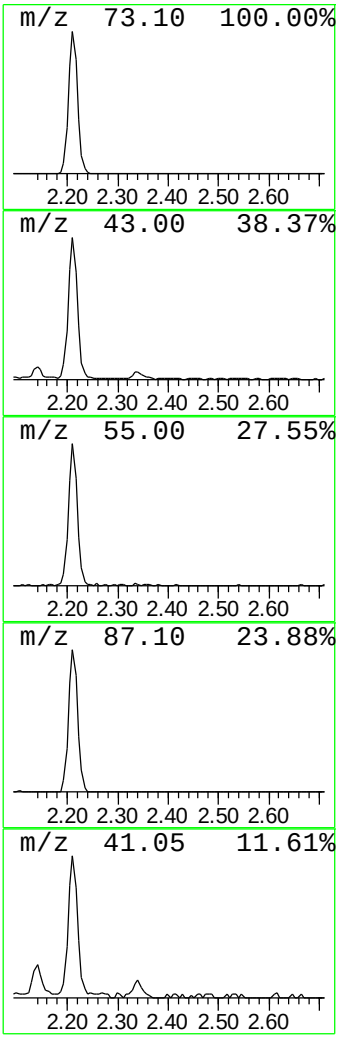
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	8.08 ng	357214	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12





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Operator : SJ/JU
Sample : I5427-03
Misc :
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Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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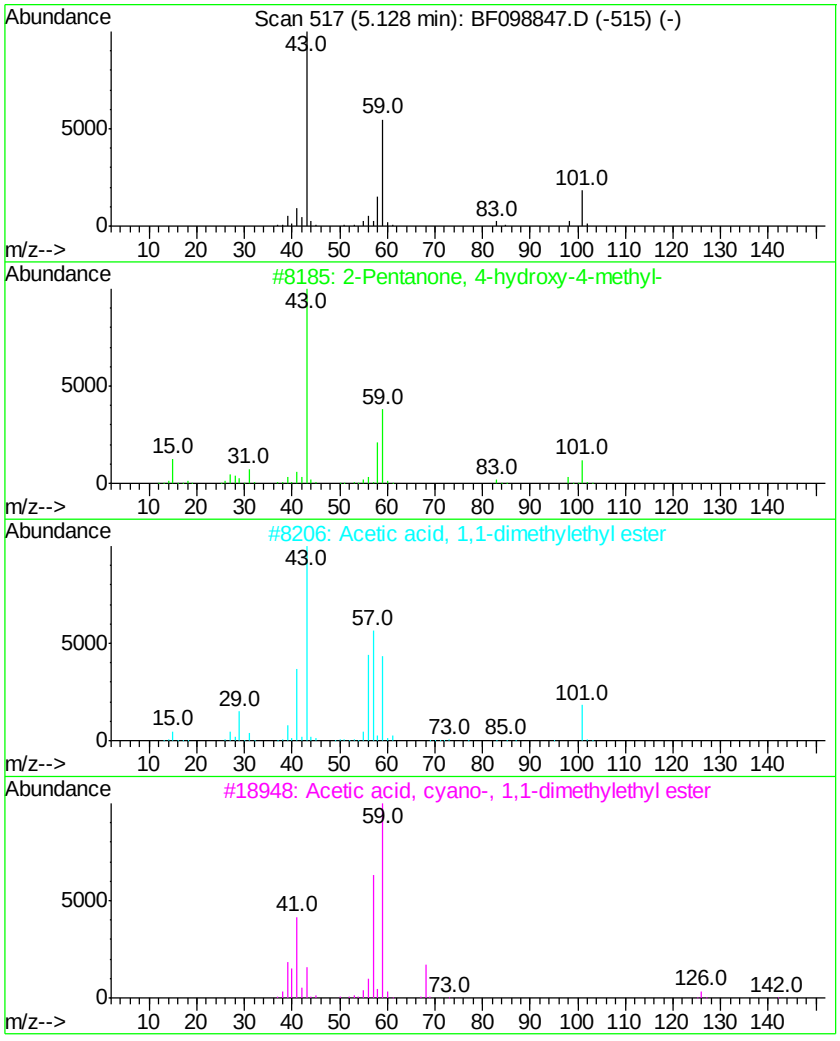
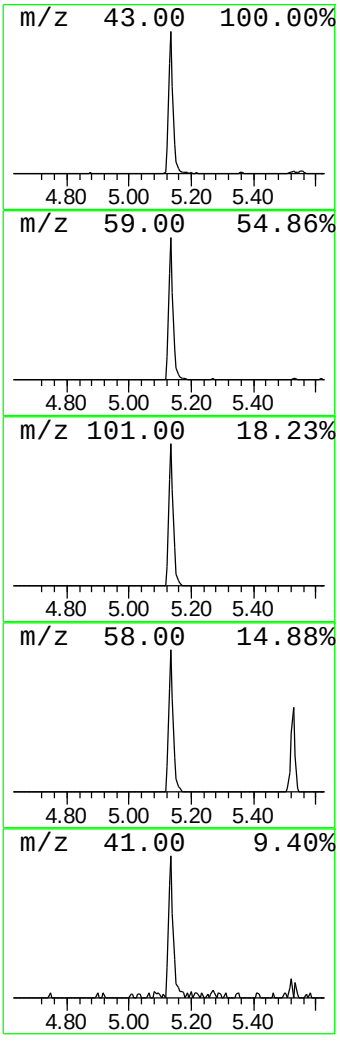
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	6.26 ng	276747	1,4-Dichlorobenzene-d4	6.91

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	37
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





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Data File : BF098847.D
Acq On : 26 Sep 2017 22:12
Operator : SJ/JU
Sample : I5427-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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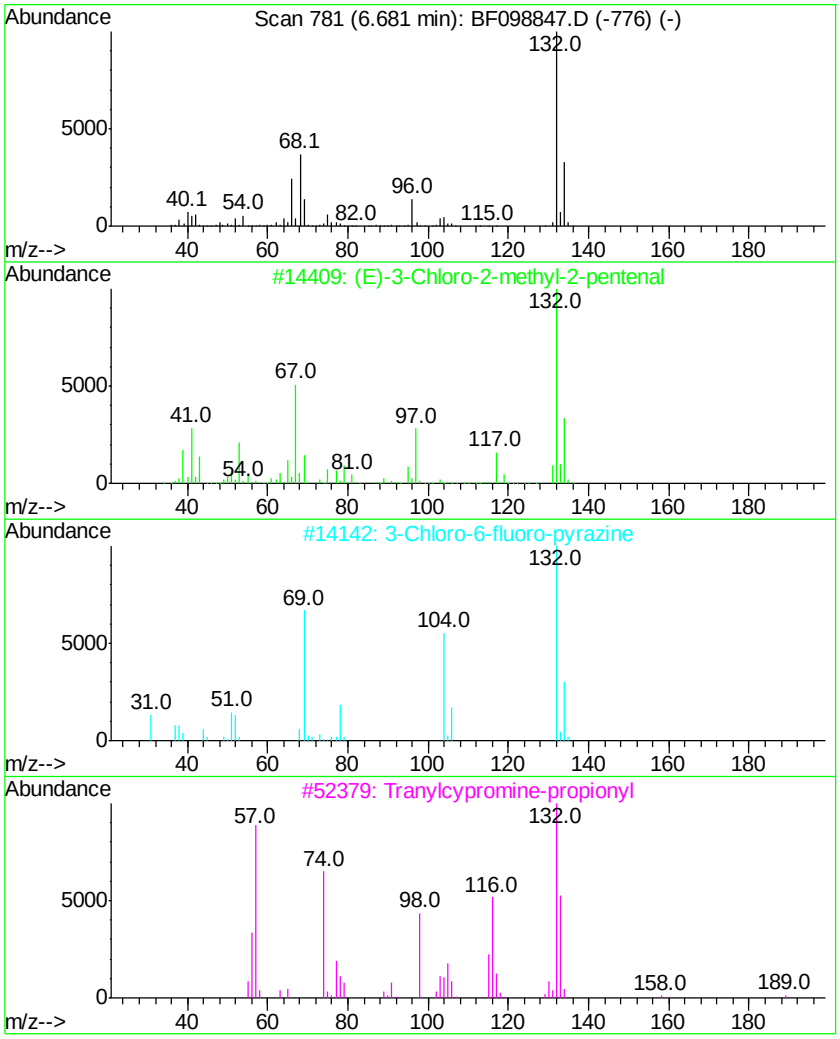
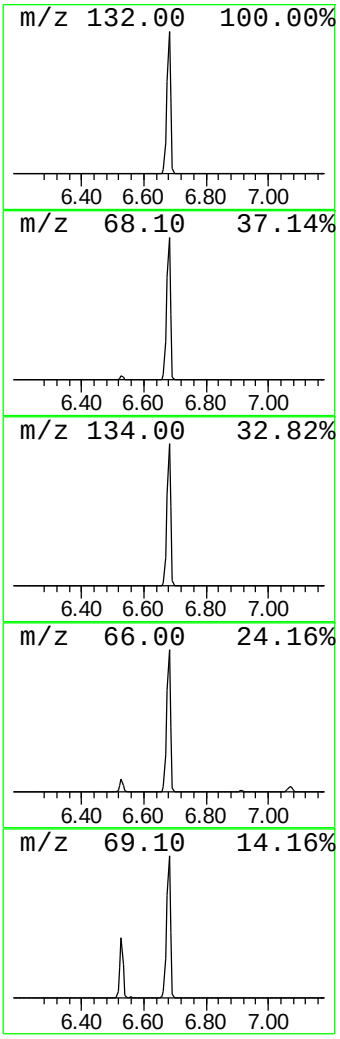
Peak Number 3 unknown6.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	58.79 ng	2598460	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092617\
Data File : BF098847.D
Acq On : 26 Sep 2017 22:12
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Sample : I5427-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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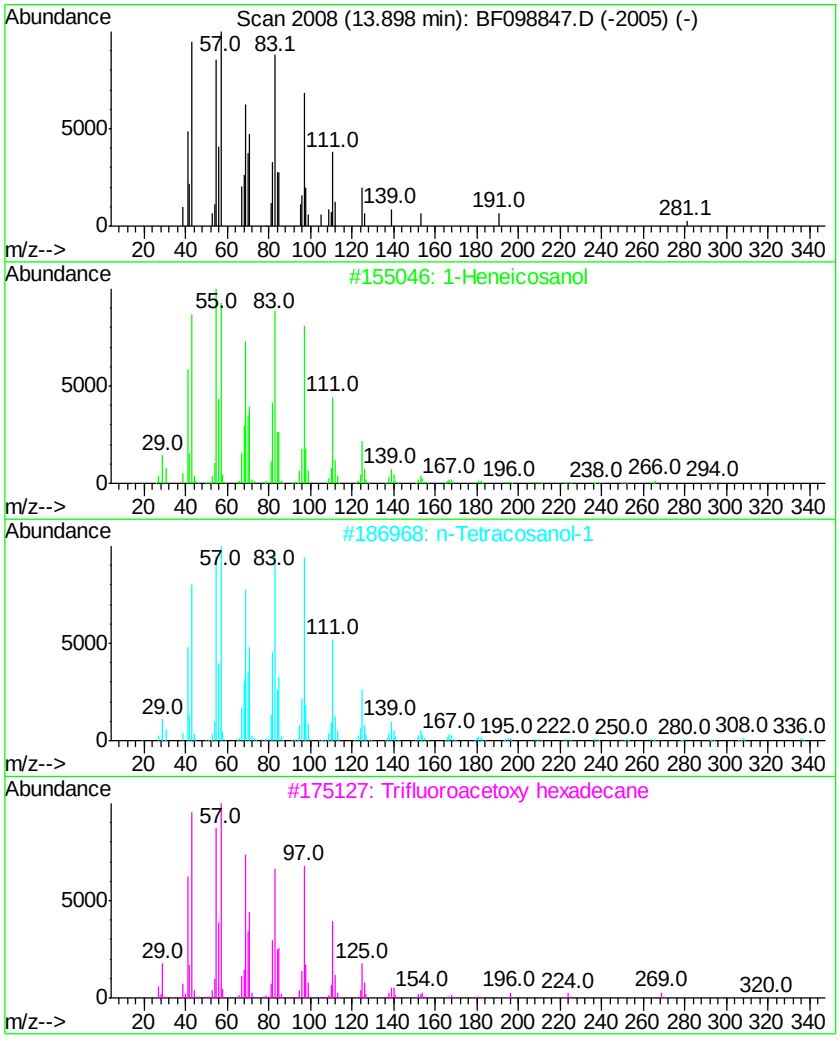
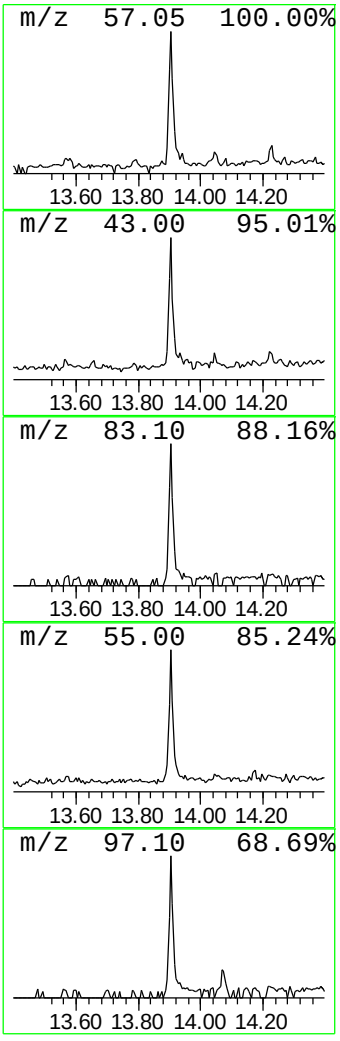
Peak Number 5 1-Heneicosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	2.11 ng	85898	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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Misc :
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Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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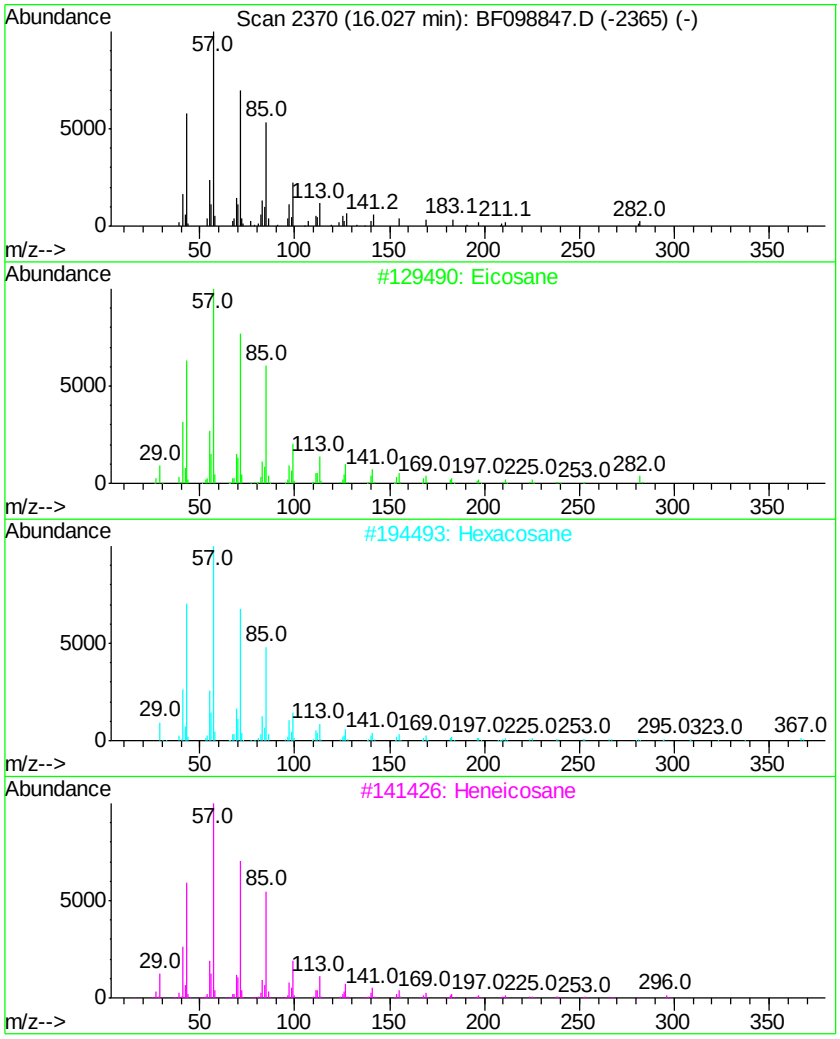
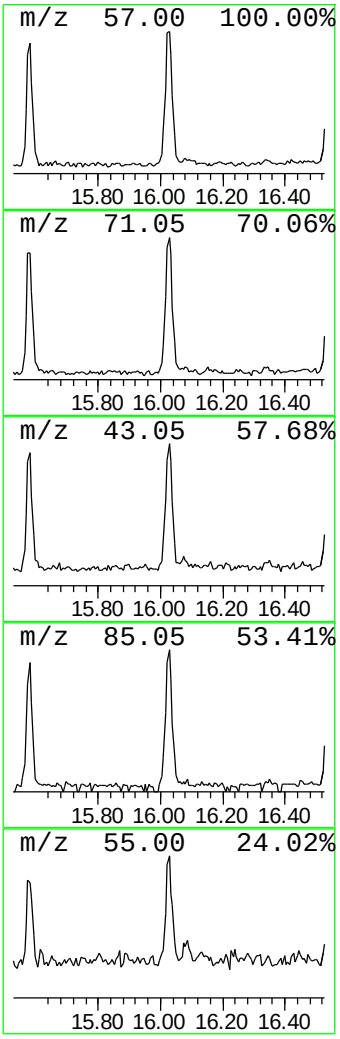
Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.70 ng	117135	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Tetracosane	338	C24H50	000646-31-1	86





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Sample : I5427-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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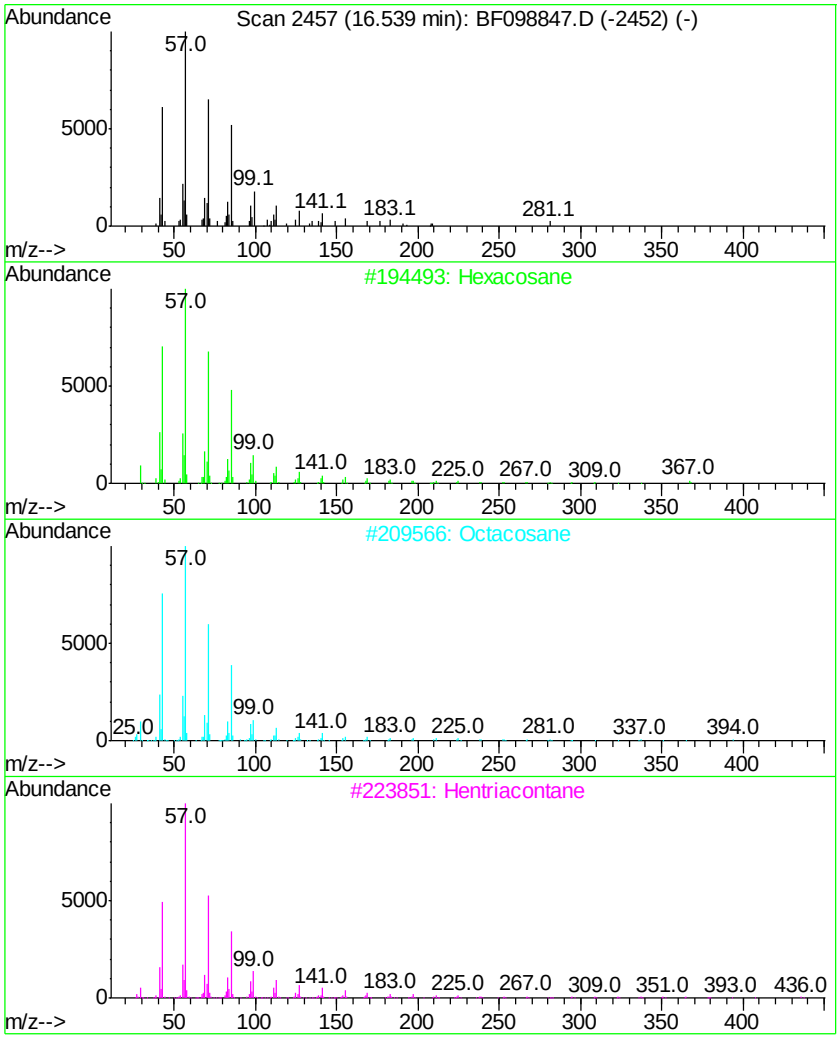
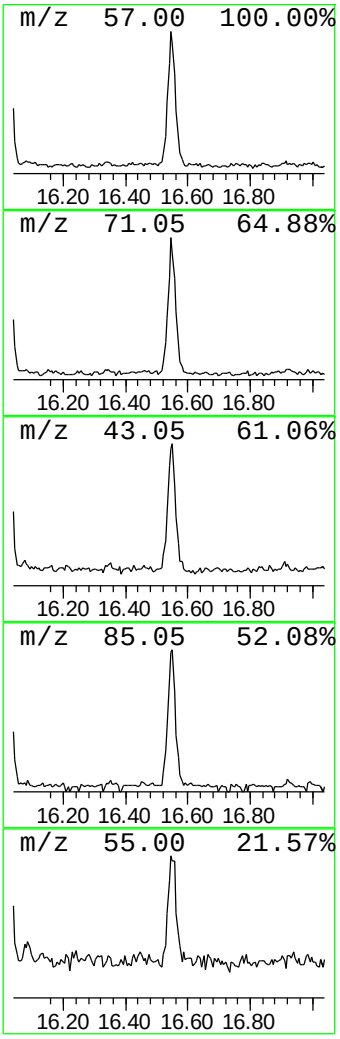
Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	3.88 ng	167985	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Misc :
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Instrument : BNA_F
ClientSampleId : 092217-SIDI-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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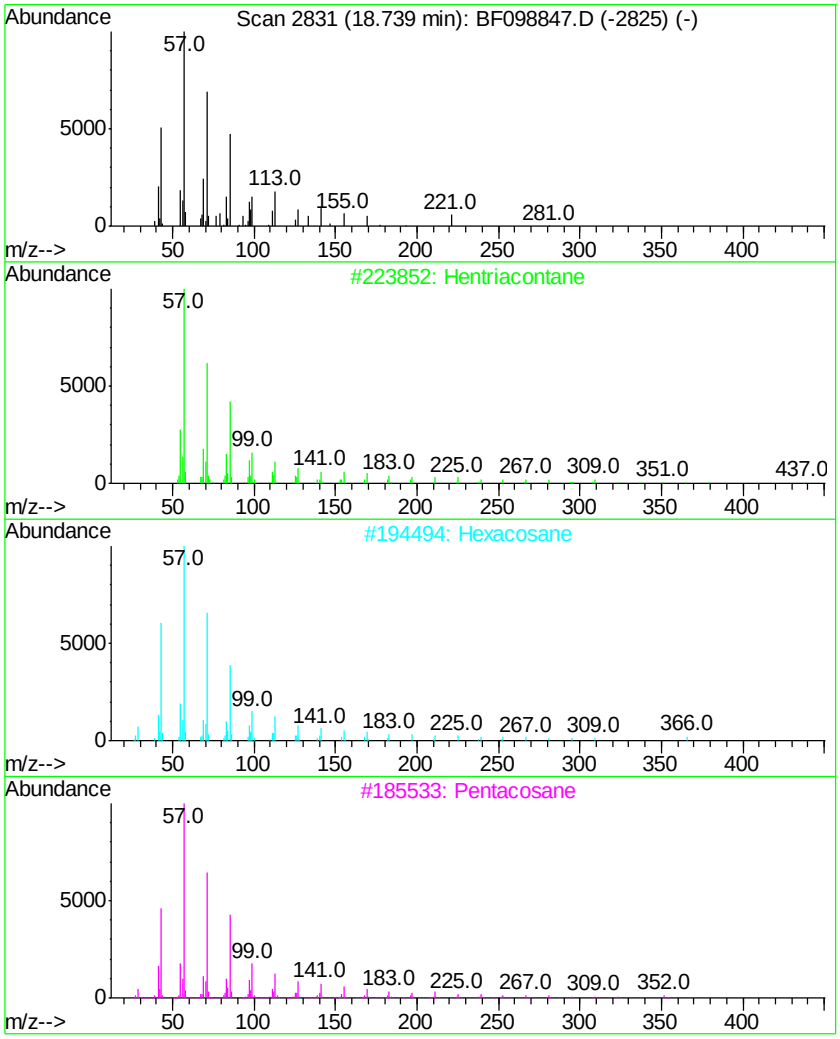
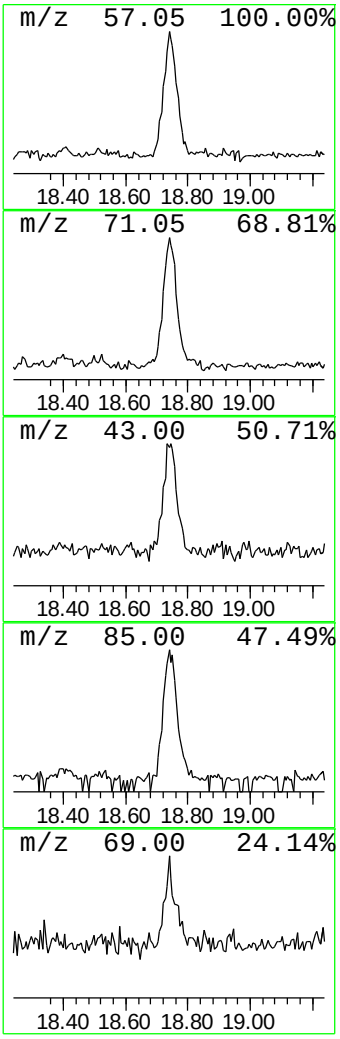
Peak Number 10 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.74	2.44 ng	105935	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Pentacosane	352	C25H52	000629-99-2	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Heptacosane	380	C27H56	000593-49-7	87





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.21	8.1	ng	357214	1	6.91	883962	20.0
2-Pentanone, 4-hy...	5.13	6.3	ng	276747	1	6.91	883962	20.0
unknown6.68	6.68	58.8	ng	2598460	1	6.91	883962	20.0
1-Heneicosanol	13.90	2.1	ng	85898	5	14.07	813999	20.0
Eicosane	16.03	2.7	ng	117135	6	15.57	866833	20.0
Hexacosane	16.54	3.9	ng	167985	6	15.57	866833	20.0
Hentriacontane	18.74	2.4	ng	105935	6	15.57	866833	20.0