LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097043.D
Acq On : 25 Jul 2017 21:49
Operator : SJ/JU
Sample : I4359-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-8-(0-2)

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-BF072517.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	2.316	68	73	80	rVB	38427	54413	1.64%	0.186%
2	4.651	467	470	487	rVB	282109	483804	14.61%	1.652%
3	5.104	542	547	565	rBV	2804031	3184380	96.13%	10.872%
4	6.169	722	728	738	rBV	2601567	3312415	100.00%	11.309%
5	6.275	741	746	749	rBV	2936648	2917731	88.08%	9.962%
6	6.498	780	784	793	rVB	892471	783630	23.66%	2.675%
7	6.657	806	811	814	rBV	2209763	2252893	68.01%	7.692%
8	6.922	850	856	861	rBV	55224	53721	1.62%	0.183%
9	7.069	875	881	884	rBV	1914261	1987596	60.00%	6.786%
10	7.781	997	1002	1006	rBV	1262124	1090096	32.91%	3.722%
11	8.863	1180	1186	1189	rBV	2931577	3125430	94.36%	10.671%
12	9.257	1249	1253	1256	rBV	413192	317133	9.57%	1.083%
13	9.528	1294	1299	1302	rBV	1302646	1232882	37.22%	4.209%
14	9.980	1373	1376	1379	rVB	113310	87185	2.63%	0.298%
15	10.198	1406	1413	1416	rBV	41541	60140	1.82%	0.205%
16	10.316	1428	1433	1436	rBV	1679751	1762320	53.20%	6.017%
17	10.451	1452	1456	1465	rBV	153104	178227	5.38%	0.609%
18	10.645	1485	1489	1492	rBV2	23447	34465	1.04%	0.118%
19	10.898	1527	1532	1534	rBV	61566	60268	1.82%	0.206%
20	10.998	1543	1549	1552	rBV	1187857	1022630	30.87%	3.491%
21	11.322	1599	1604	1609	rBV2	27809	35888	1.08%	0.123%
22	11.557	1640	1644	1651	rBV2	280117	282104	8.52%	0.963%
23	12.333	1773	1776	1782	rBV	71801	83436	2.52%	0.285%
24	12.586	1814	1819	1822	rBV	2443467	2630344	79.41%	8.981%
25	13.492	1969	1973	1981	rBV	281849	309502	9.34%	1.057%
26	13.621	1990	1995	2003	rBV	909503	906214	27.36%	3.094%
27	13.816	2025	2028	2034	rBV3	21891	33572	1.01%	0.115%
28	14.121	2077	2080	2088	rBV	68109	87892	2.65%	0.300%
29	14.704	2176	2179	2185	rBV	75367	94833	2.86%	0.324%
30	14.968	2219	2224	2230	rBV	566818	626315	18.91%	2.138%
31	15.380	2290	2294	2298	rBV	62105	91972	2.78%	0.314%
32	15.415	2298	2300	2306	rVB3	36721	51686	1.56%	0.176%
33	16.662	2507	2512	2518	rVB8	26137	54171	1.64%	0.185%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097043.D
Acq On : 25 Jul 2017 21:49
Operator : SJ/JU
Sample : I4359-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-8-(0-2)

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

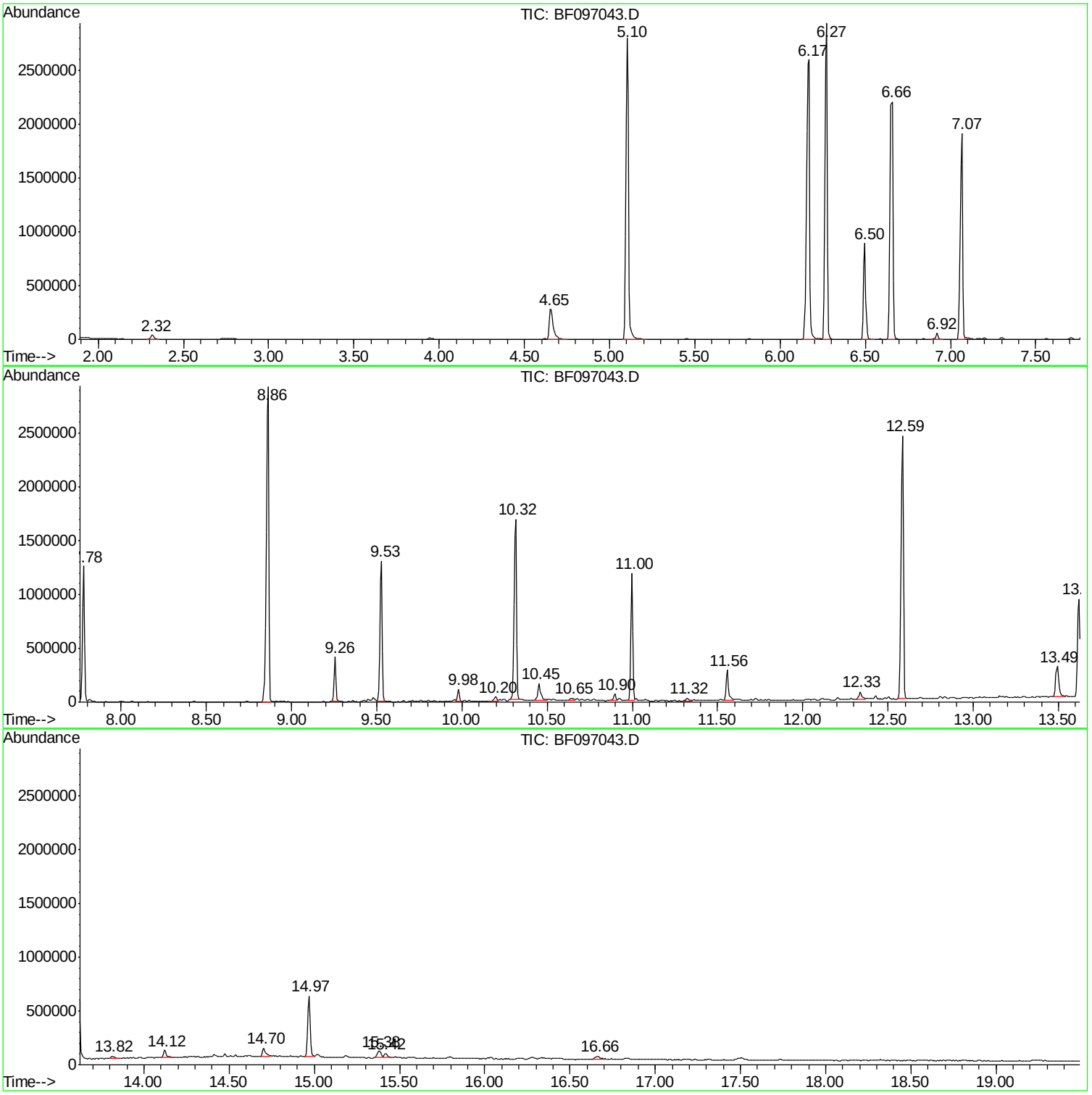
Sum of corrected areas: 29289288

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097043.D
Acq On : 25 Jul 2017 21:49
Operator : SJ/JU
Sample : I4359-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-8-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097043.D
Acq On : 25 Jul 2017 21:49
Operator : SJ/JU
Sample : I4359-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-8-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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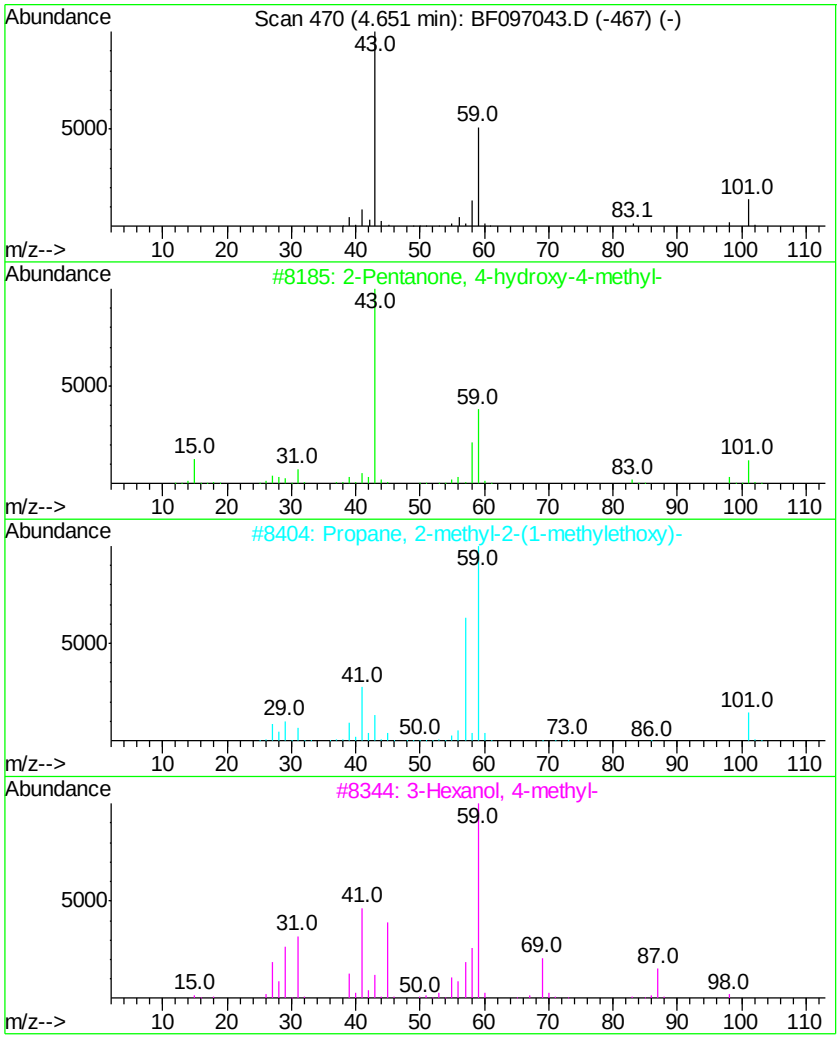
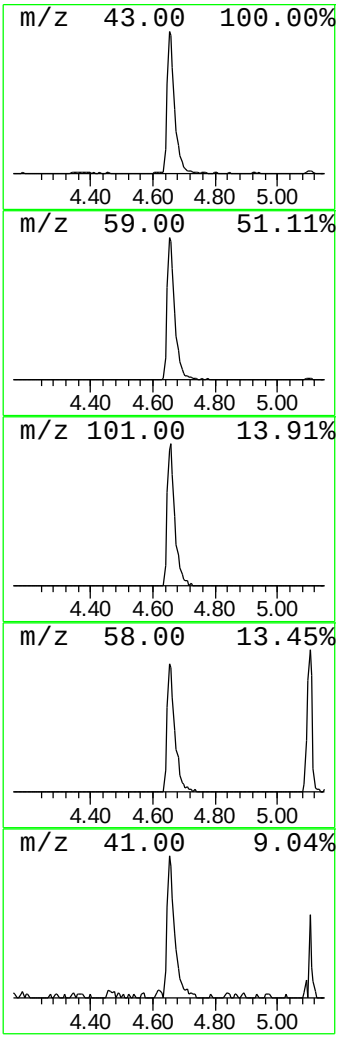
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	12.35 ng	483804	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Hexanol	102	C6H14O	000623-37-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097043.D
Acq On : 25 Jul 2017 21:49
Operator : SJ/JU
Sample : I4359-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-8-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

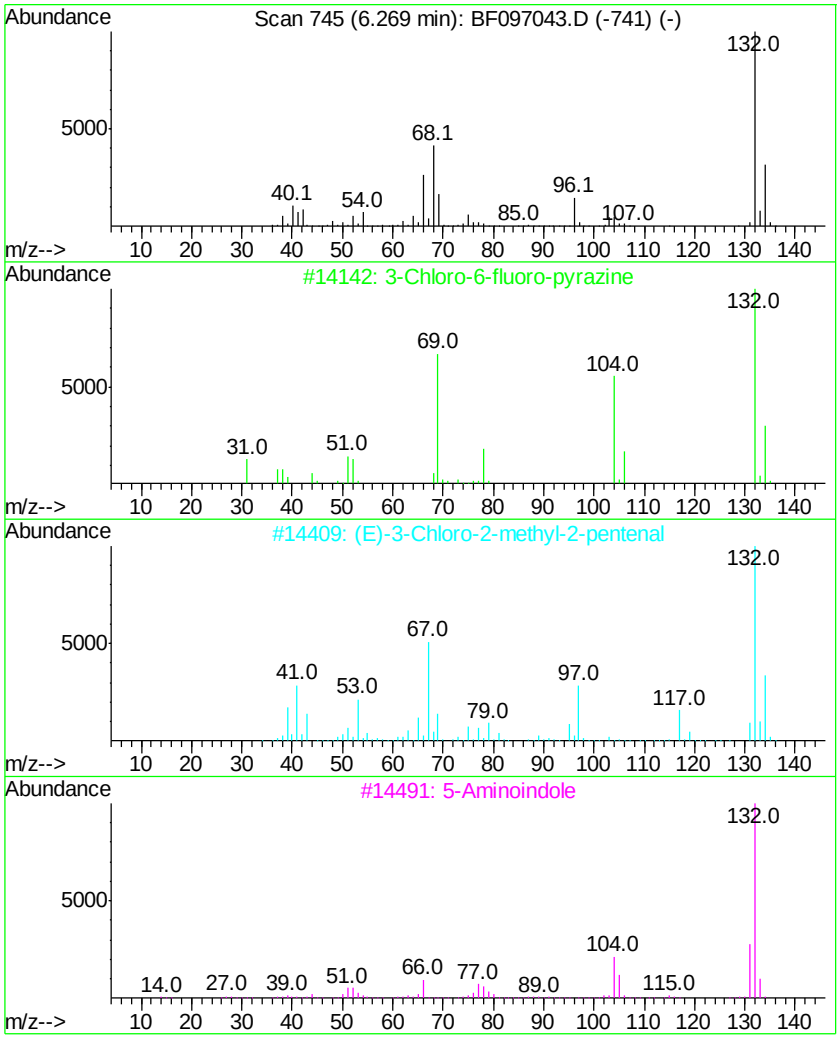
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

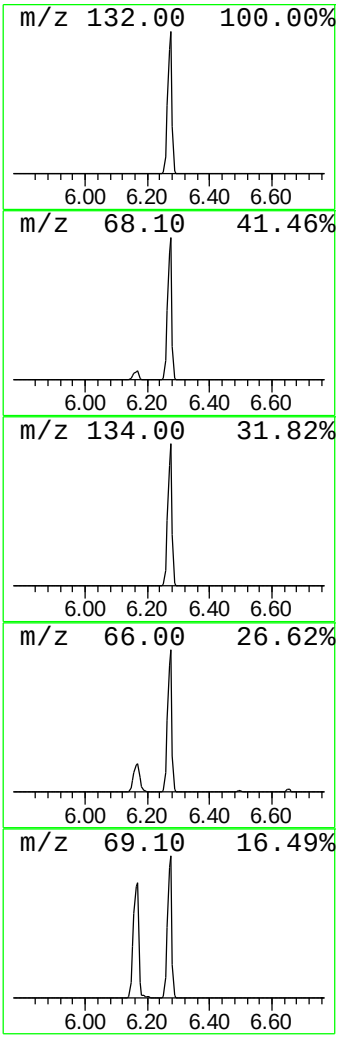
****

Peak Number 2 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	74.47 ng	2917730	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Operator : SJ/JU
Sample : I4359-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-8-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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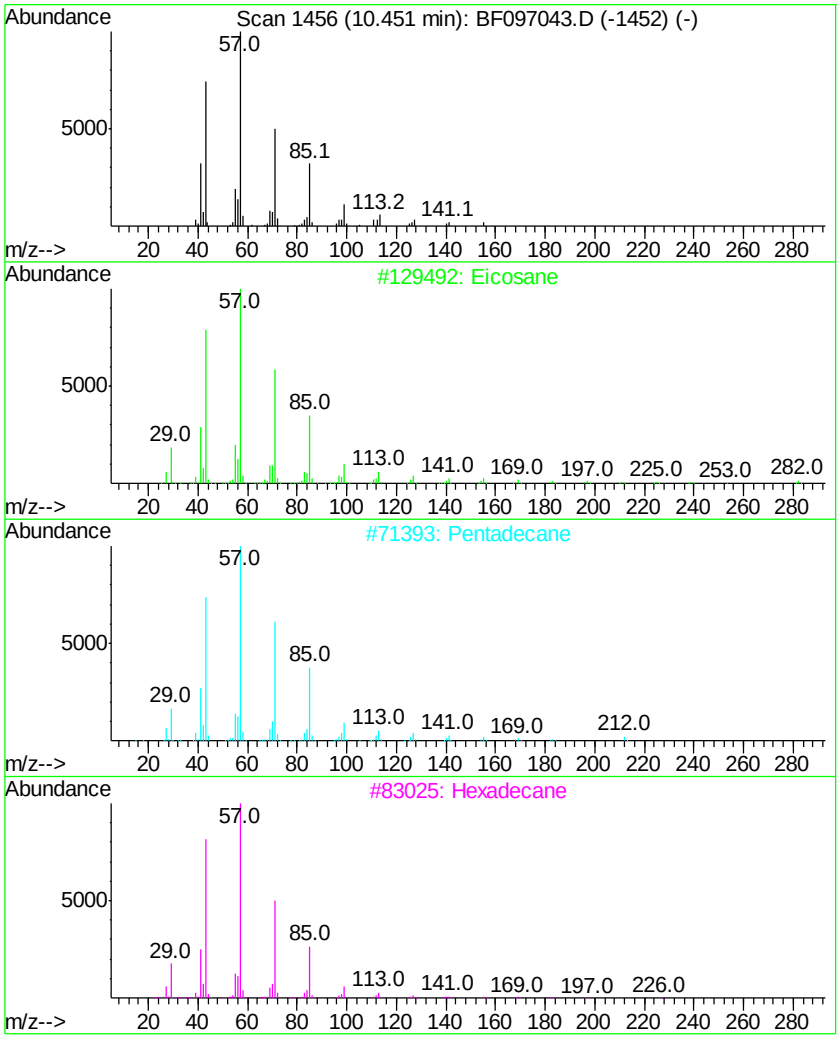
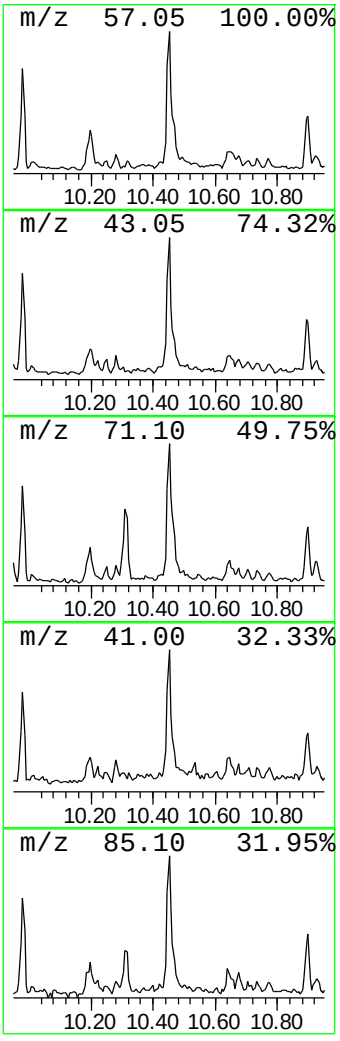
Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	3.49 ng	178227	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Pentadecane	212	C15H32	000629-62-9	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tridecane	184	C13H28	000629-50-5	86
5	Heneicosane	296	C21H44	000629-94-7	80





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Operator : SJ/JU
Sample : I4359-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-8-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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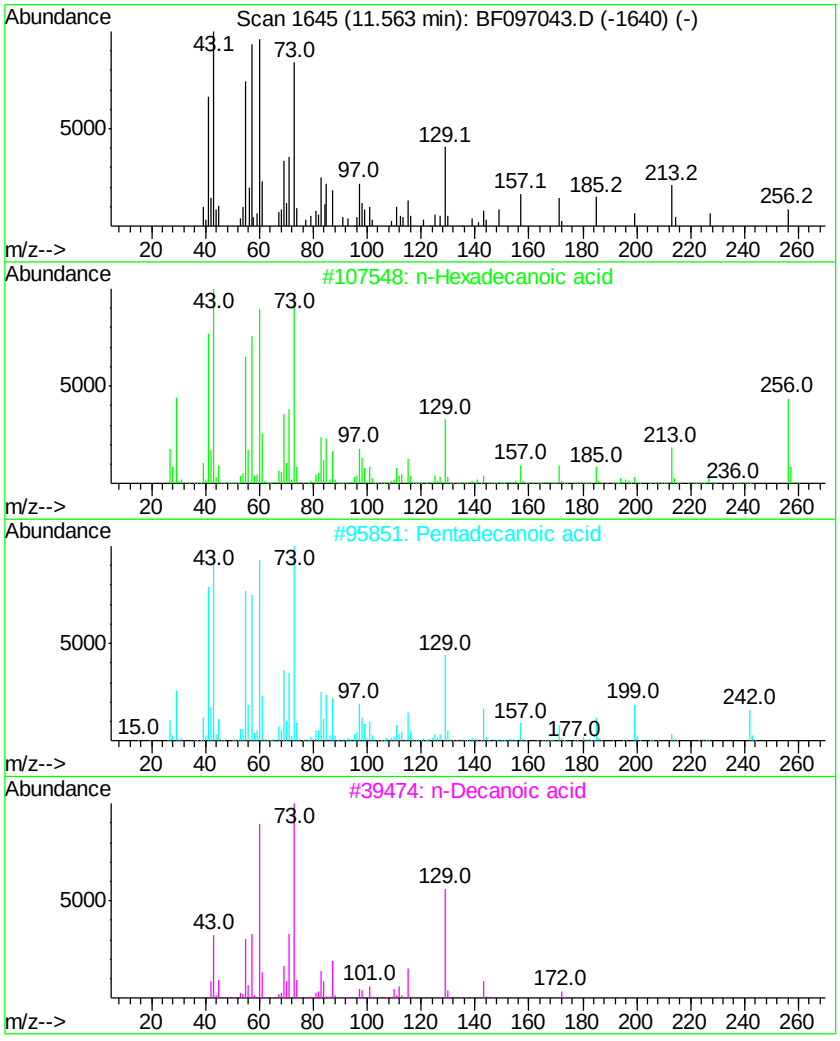
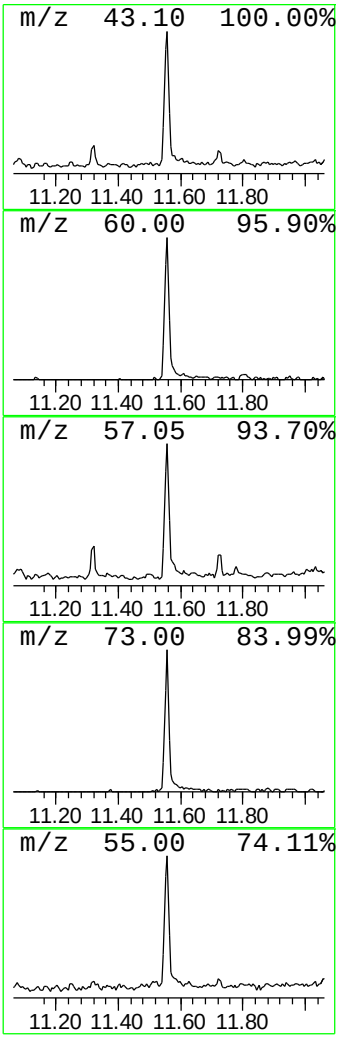
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	5.52 ng	282104	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	n-Decanoic acid	172	C10H20O2	000334-48-5	78
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Sample : I4359-15
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CEMETERY-8-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

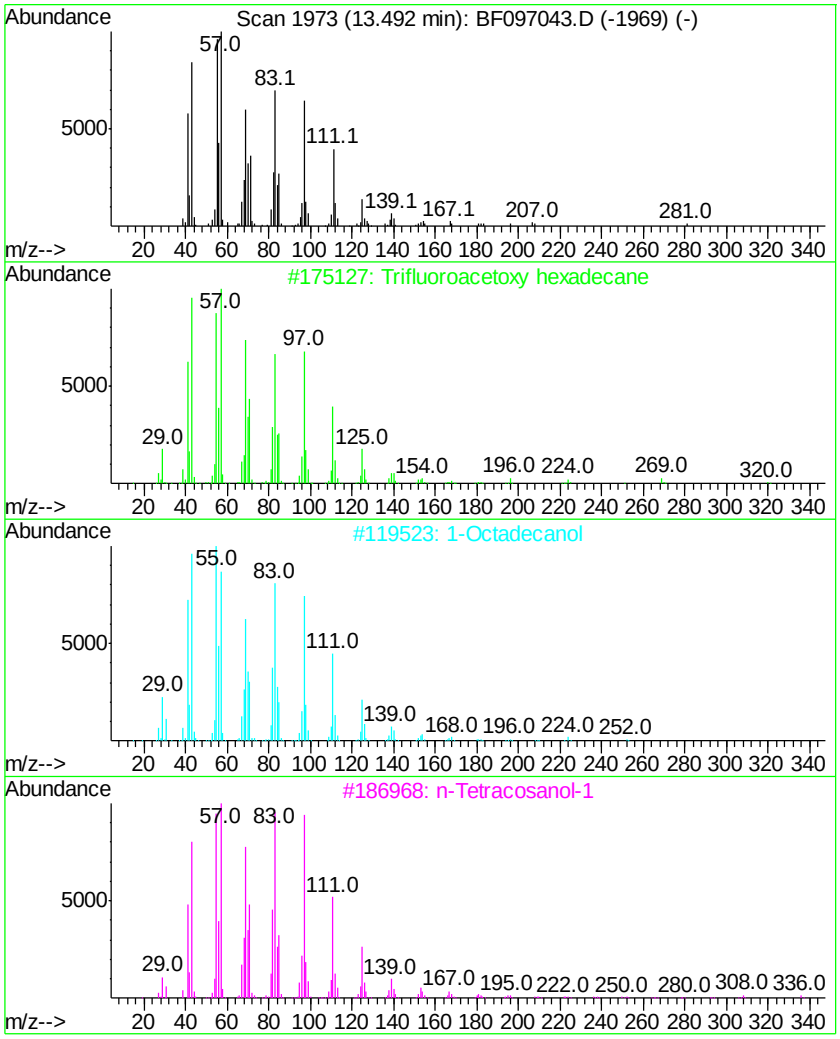
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

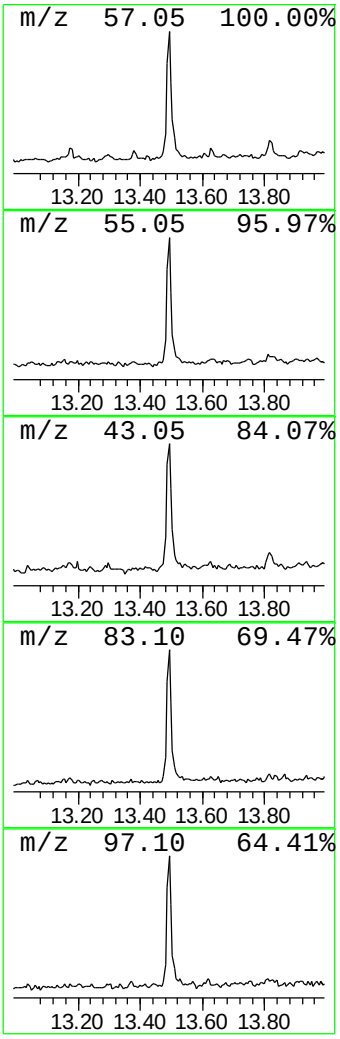
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	6.83 ng	309502	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	1-Octadecanol	270	C18H38O	000112-92-5	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	87





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Misc :
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Instrument : BNA_F
ClientSampleId : CEMETERY-8-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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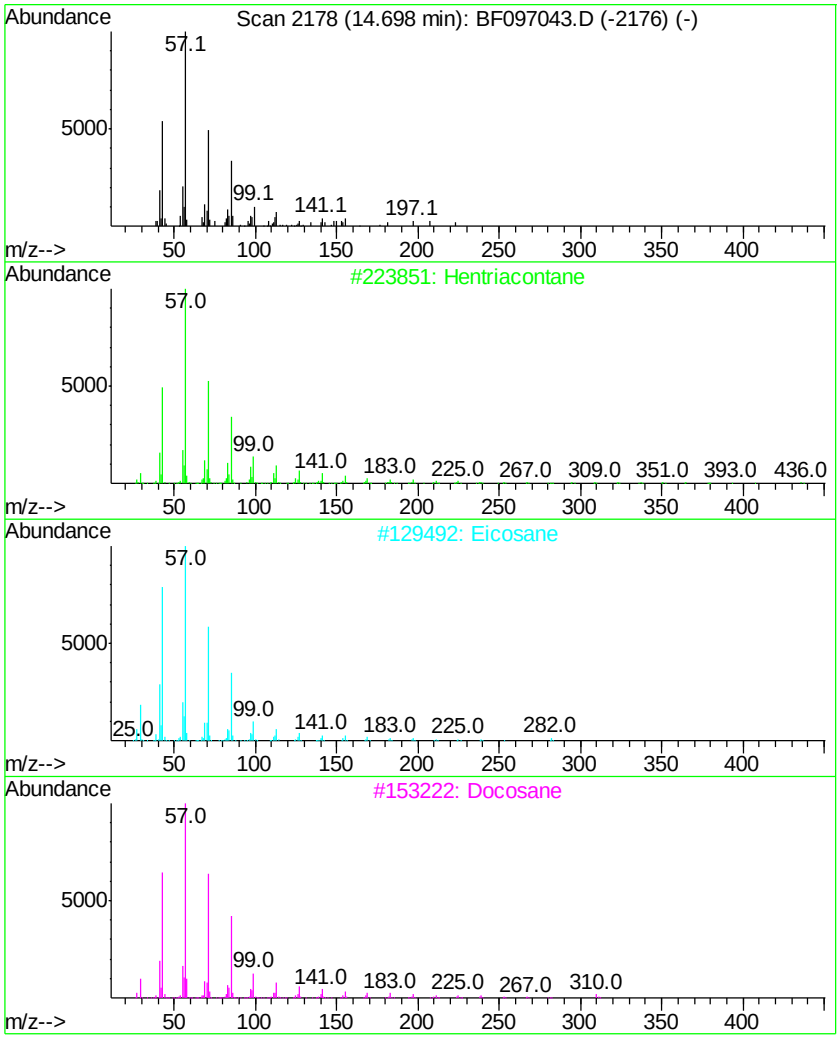
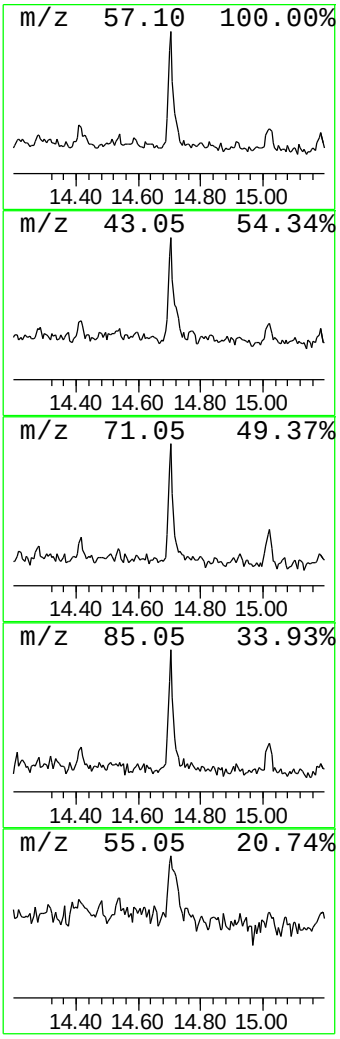
Peak Number 7 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	3.03 ng	94833	Perylene-d12	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Eicosane	282	C20H42	000112-95-8	86
3	Docosane	310	C22H46	000629-97-0	86
4	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	86
5	Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	83





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

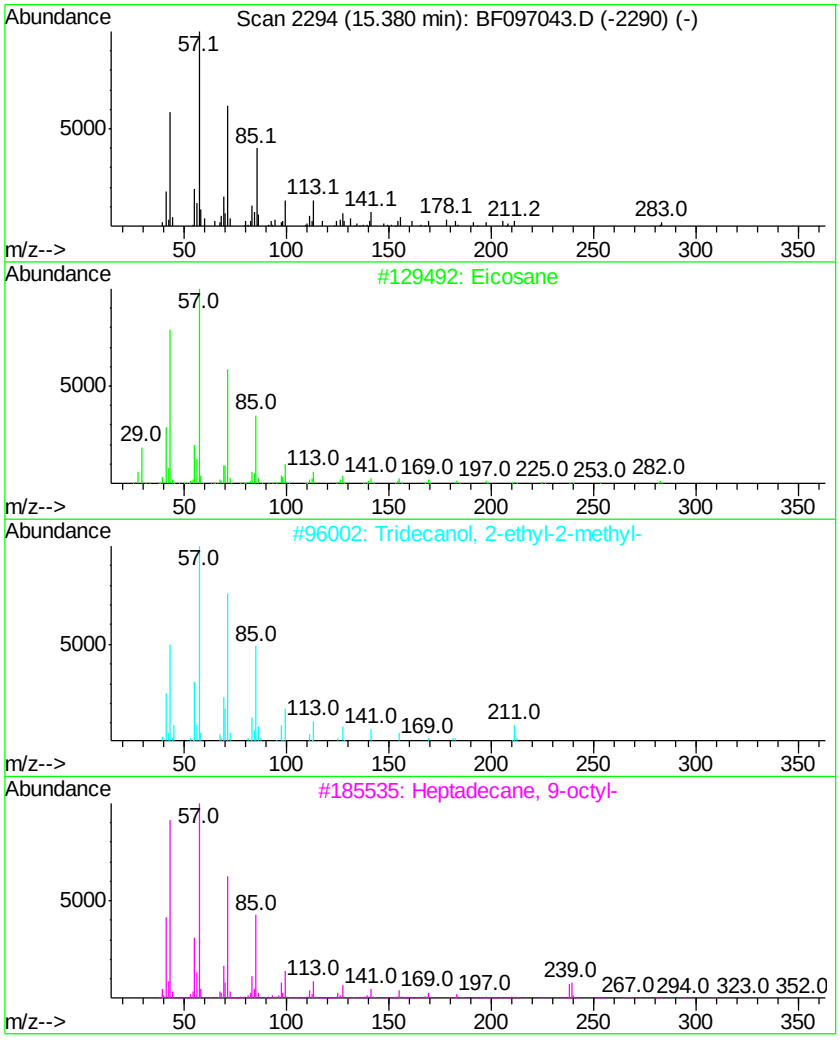
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

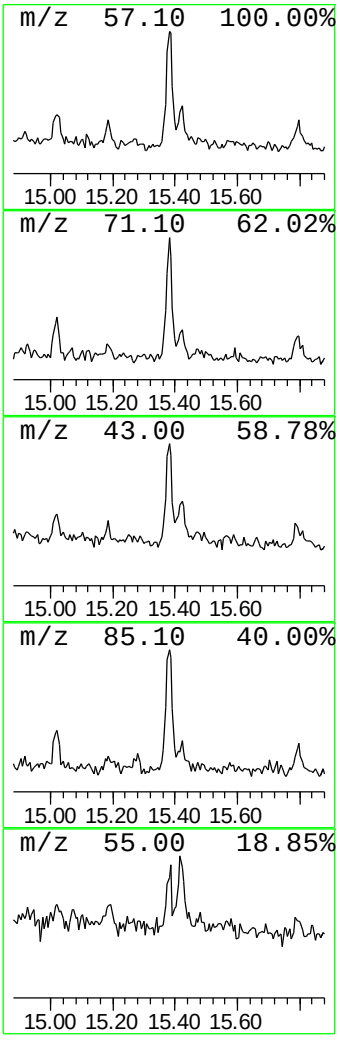
****

Peak Number 8 Tridecanol, 2-ethyl-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.38	2.94 ng	91972	Perylene-d12	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	87
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Pentacosane	352	C25H52	000629-99-2	87
5	Hentriacontane	437	C31H64	000630-04-6	87





Tentatively Identified Compound (LSC) summary

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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...	4.65	12.4	ng	483804	1	6.50	783630	20.0
unknown6.27	6.27	74.5	ng	2917730	1	6.50	783630	20.0
Eicosane	10.45	3.5	ng	178227	4	11.00	1022630	20.0
n-Hexadecanoic acid	11.56	5.5	ng	282104	4	11.00	1022630	20.0
Trifluoroacetoxy ...	13.49	6.8	ng	309502	5	13.62	906214	20.0
Hentriacontane	14.70	3.0	ng	94833	6	14.97	626315	20.0
Tridecanol, 2-eth...	15.38	2.9	ng	91972	6	14.97	626315	20.0