LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097037.D
Acq On : 25 Jul 2017 19:02
Operator : SJ/JU
Sample : I4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3-20170720

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	4.634	464	467	475	rBV	73989	95500	3.16%	0.447%
2	5.092	542	545	558	rBV	1084294	1201295	39.80%	5.621%
3	6.157	722	726	741	rBV	838292	845615	28.01%	3.957%
4	6.269	741	745	749	rBV	2407350	2196871	72.78%	10.280%
5	6.498	780	784	791	rBV	794862	722072	23.92%	3.379%
6	6.651	806	810	814	rBV	2034852	1967692	65.19%	9.208%
7	7.069	876	881	884	rBV	1708808	1798184	59.57%	8.414%
8	7.780	998	1002	1010	rVB	1200873	1003772	33.25%	4.697%
9	8.863	1180	1186	1189	rBV	2933225	3018623	100.00%	14.125%
10	9.027	1210	1214	1219	rVB	32325	32249	1.07%	0.151%
11	9.257	1250	1253	1256	rBV	93106	69624	2.31%	0.326%
12	9.527	1294	1299	1302	rBV	1053480	986980	32.70%	4.619%
13	10.316	1428	1433	1436	rBV	1641444	1684704	55.81%	7.883%
14	10.404	1444	1448	1453	rBV	111030	96152	3.19%	0.450%
15	10.451	1453	1456	1463	rVB	35542	40355	1.34%	0.189%
16	10.998	1545	1549	1553	rBV	1074474	919003	30.44%	4.300%
17	11.557	1640	1644	1646	rBV	93391	93940	3.11%	0.440%
18	11.586	1646	1649	1656	rVB2	129312	142724	4.73%	0.668%
19	12.333	1774	1776	1780	rBV4	49448	48535	1.61%	0.227%
20	12.586	1814	1819	1822	rBV2	2444026	2675971	88.65%	12.522%
21	12.633	1822	1827	1833	rVB	122657	135291	4.48%	0.633%
22	13.492	1970	1973	1979	rVV	63314	71020	2.35%	0.332%
23	13.557	1981	1984	1991	rVV	99658	104824	3.47%	0.491%
24	13.621	1991	1995	2003	rVB	887138	830456	27.51%	3.886%
25	14.386	2121	2125	2136	rBV	49134	69248	2.29%	0.324%
26	14.968	2220	2224	2231	rBV	477920	519365	17.21%	2.430%

Sum of corrected areas: 21370065

LSC Report - Integrated Chromatogram

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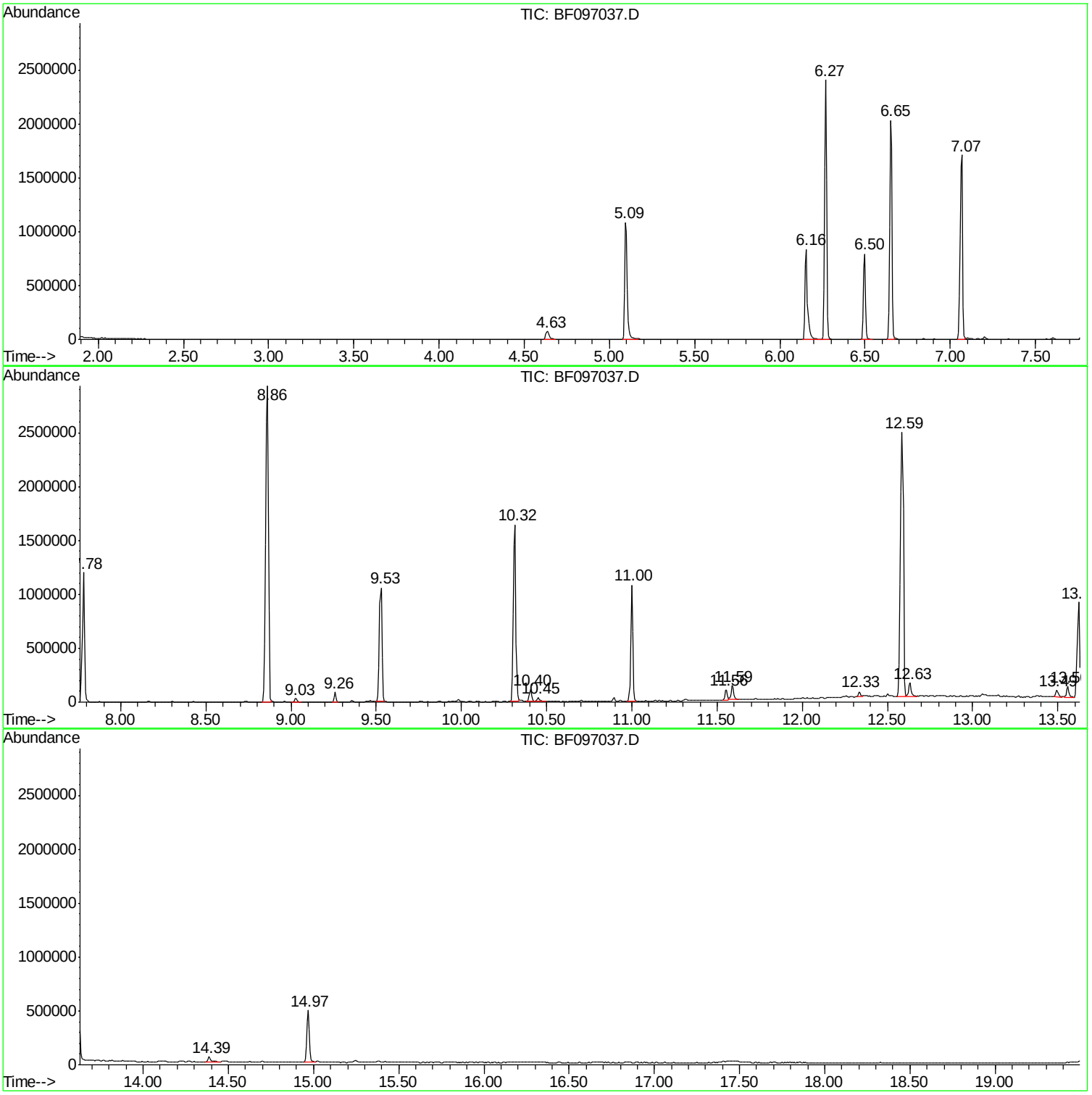
Operator : SJ/JU
Sample : I4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3-20170720

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097037.D
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Operator : SJ/JU
Sample : I4369-03
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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3-20170720

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

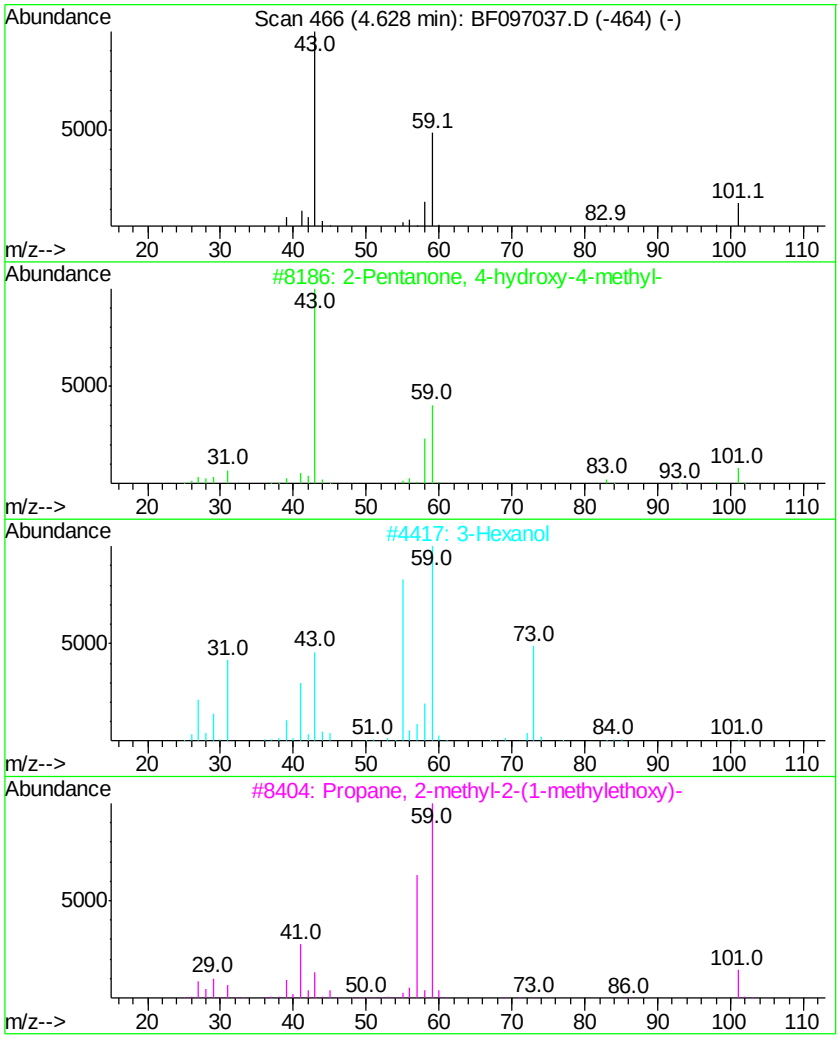
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

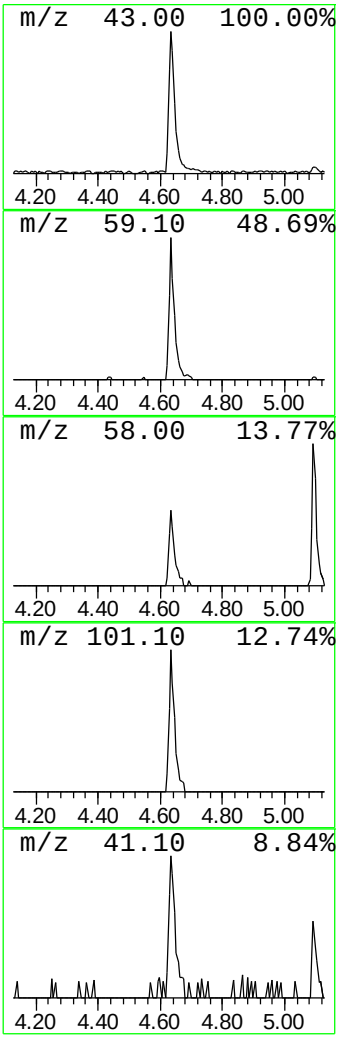
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	2.65 ng	95500	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	50
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Library Search Compound Report

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Data File : BF097037.D
Acq On : 25 Jul 2017 19:02
Operator : SJ/JU
Sample : I4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3-20170720

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

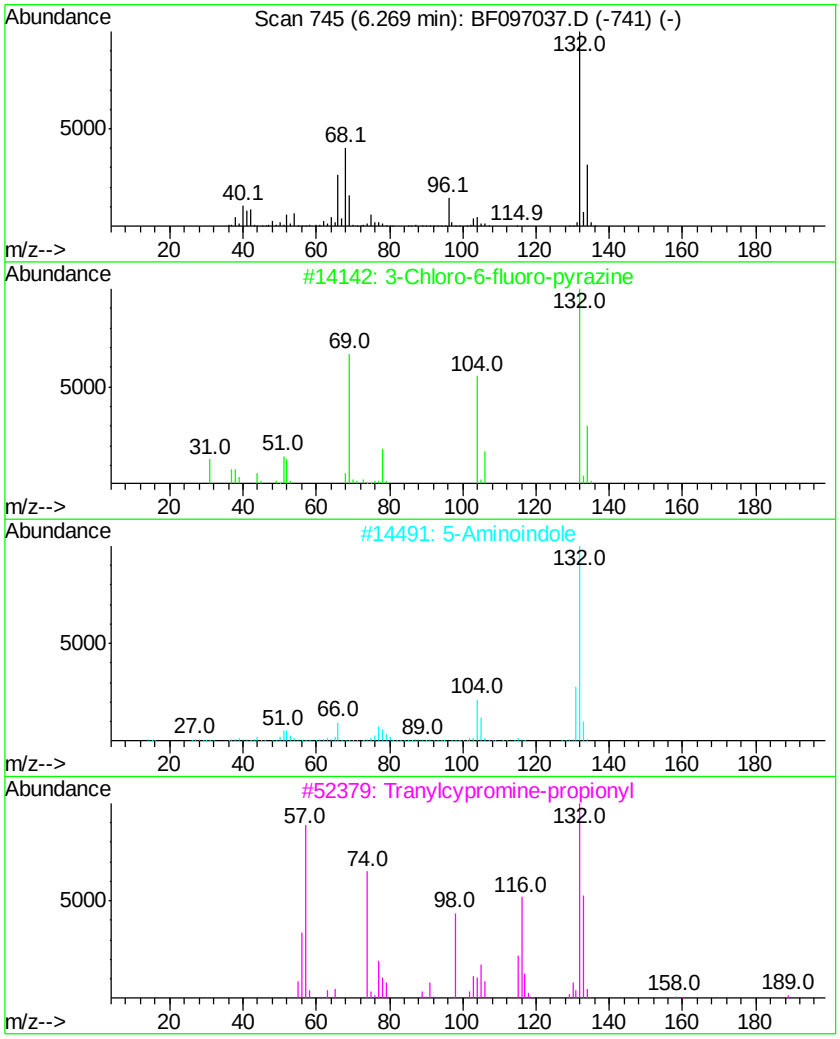
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

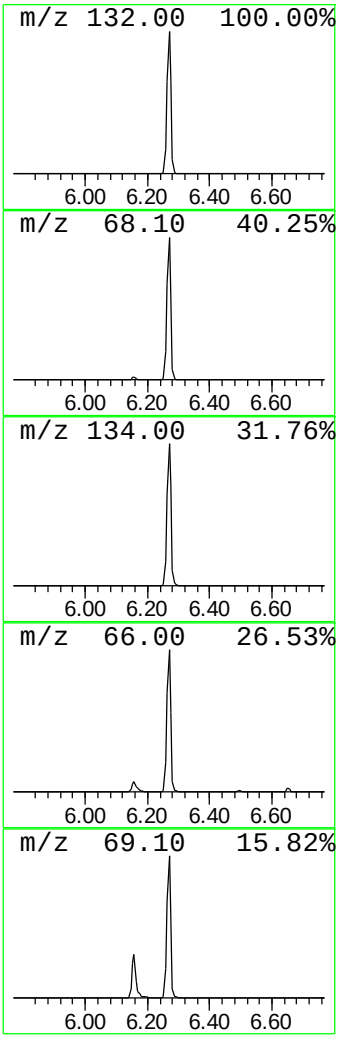
****

Peak Number 2 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	60.85 ng	2196870	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	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Data File : BF097037.D
Acq On : 25 Jul 2017 19:02
Operator : SJ/JU
Sample : I4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3-20170720

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

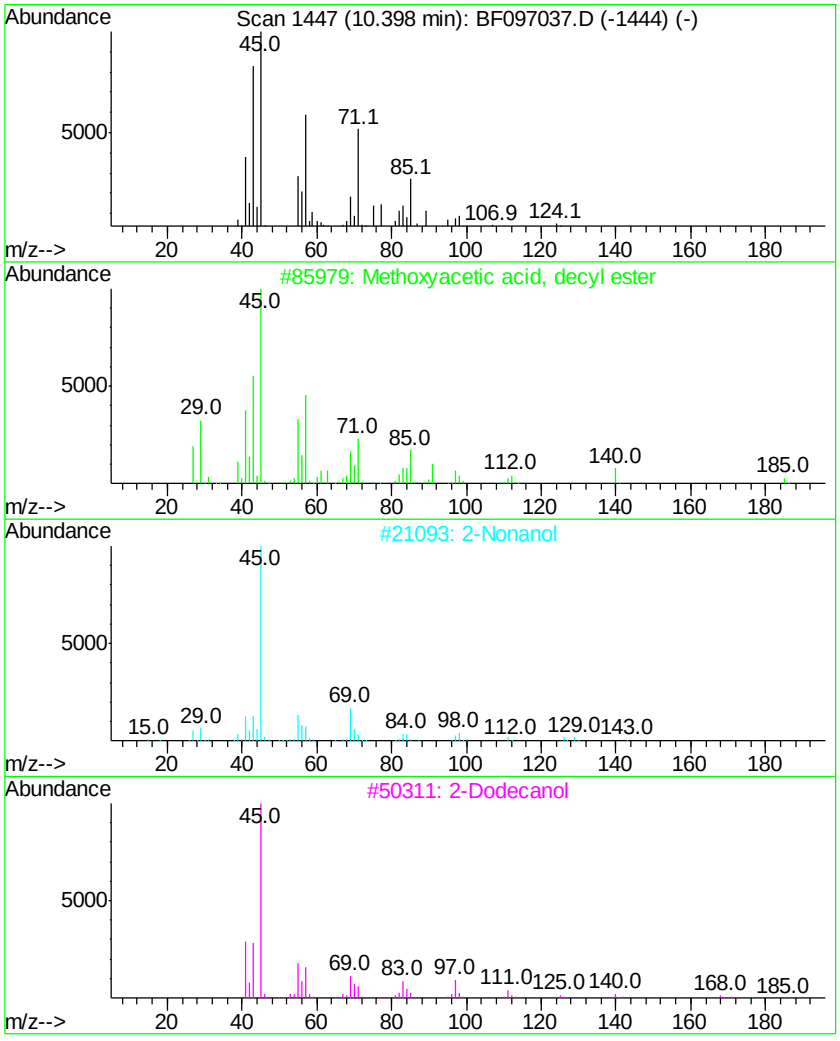
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

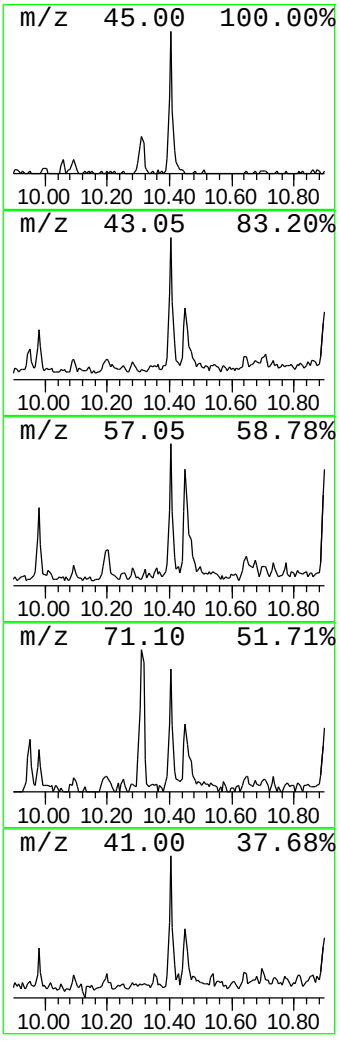
****

Peak Number 4 Methoxyacetic acid, decyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	2.09 ng	96152	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, decyl ester	230	C13H26O3	259141-02-1	53
2	2-Nonanol	144	C9H20O	000628-99-9	38
3	2-Dodecanol	186	C12H26O	010203-28-8	38
4	2-Octanol	130	C8H18O	000123-96-6	35
5	Diethylene glycol hexyl ether	190	C10H22O3	000112-59-4	27





Library Search Compound Report

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Data File : BF097037.D
Acq On : 25 Jul 2017 19:02
Operator : SJ/JU
Sample : I4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3-20170720

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

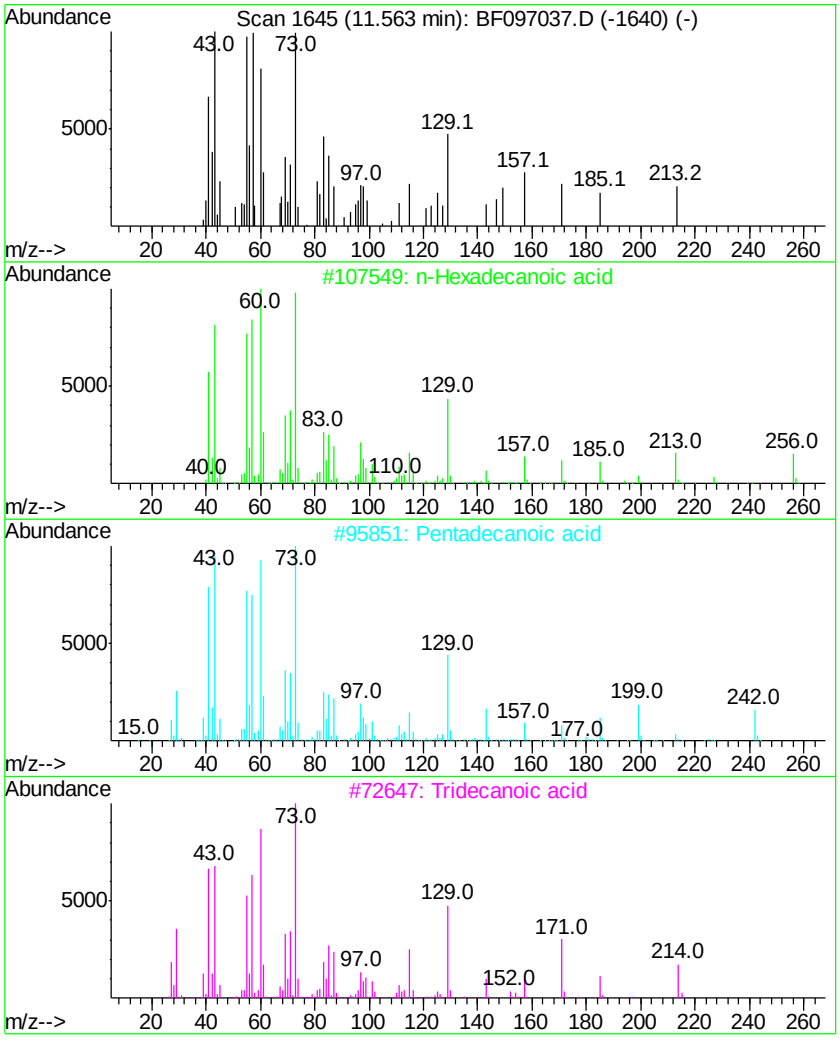
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

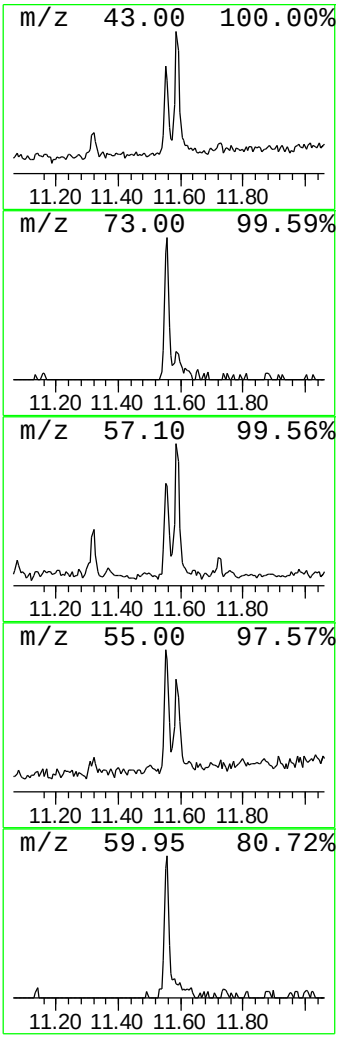
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	2.04 ng	93940	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Trehalose	342	C12H22O11	000099-20-7	53





Library Search Compound Report

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Sample : I4369-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3-20170720

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

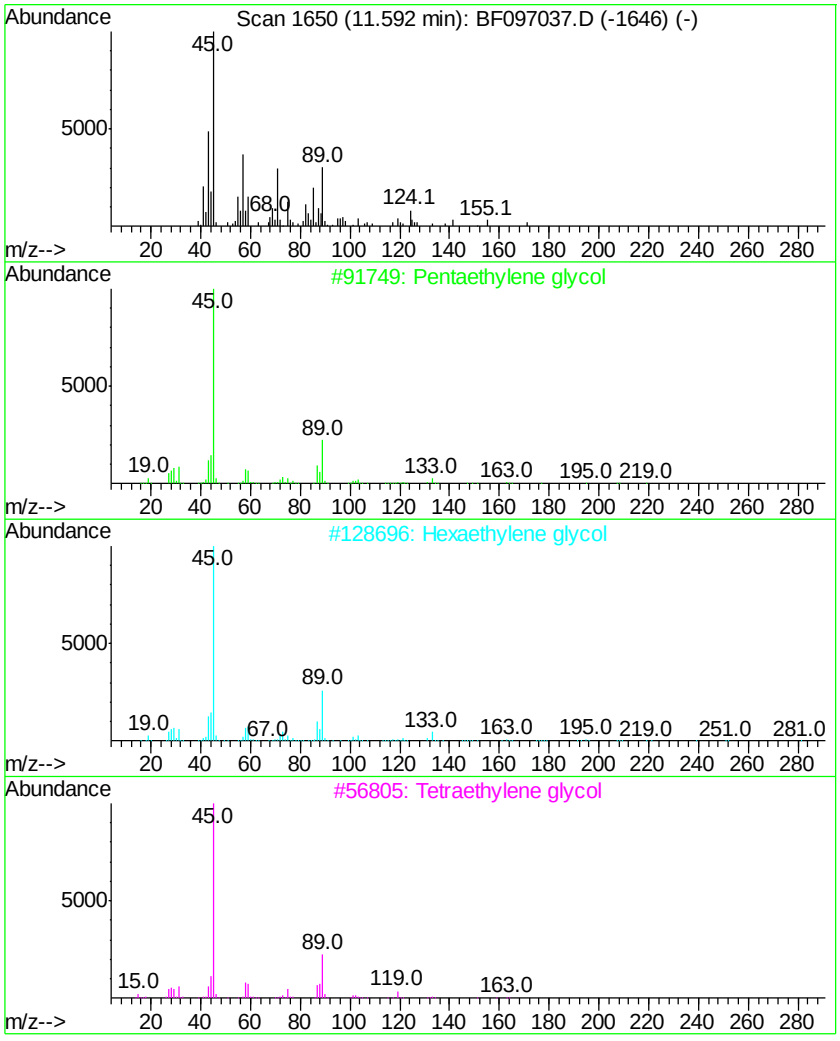
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

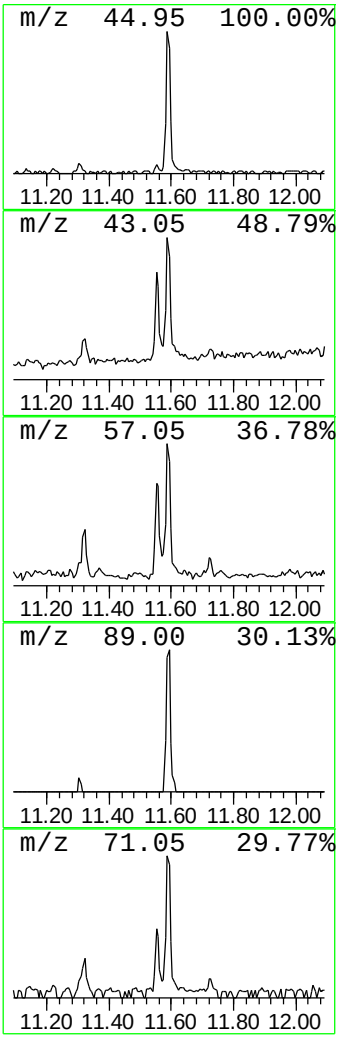
****

Peak Number 6 Pentaethylene glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	3.11 ng	142724	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	59
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	58
3	Tetraethylene glycol	194	C8H18O5	000112-60-7	53
4	Triethylene glycol monododecyl e...	318	C18H38O4	003055-94-5	50
5	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	47





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3-20170720

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

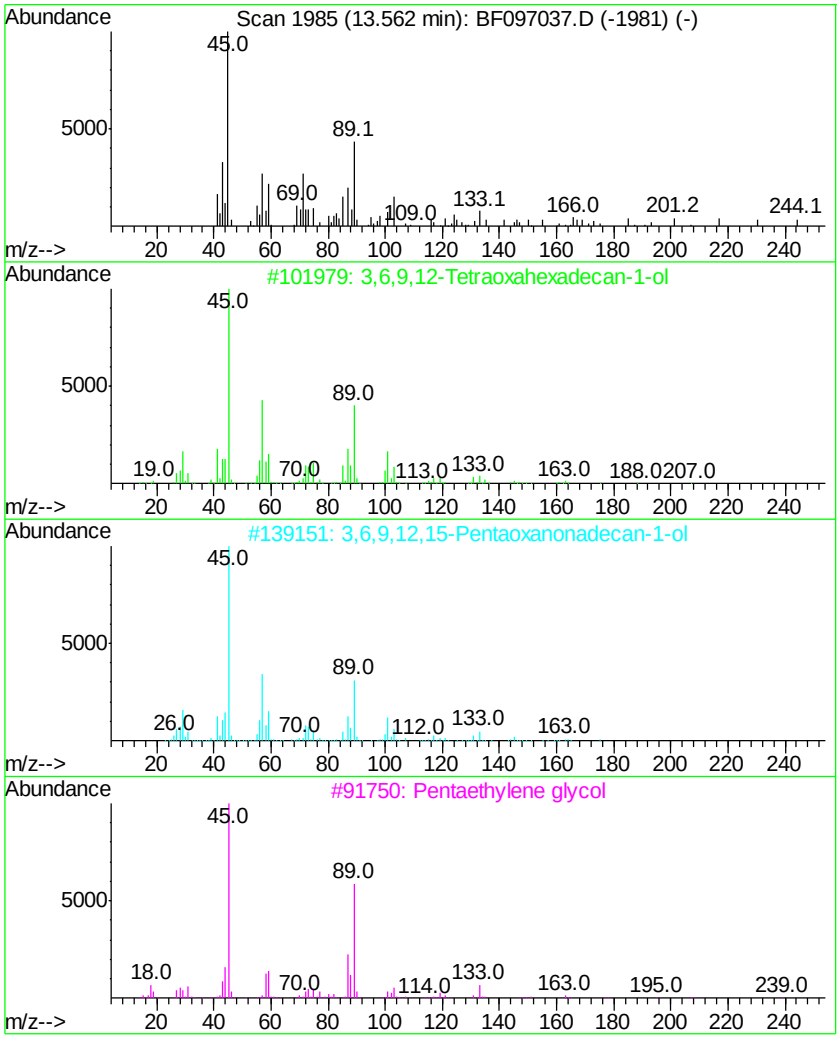
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

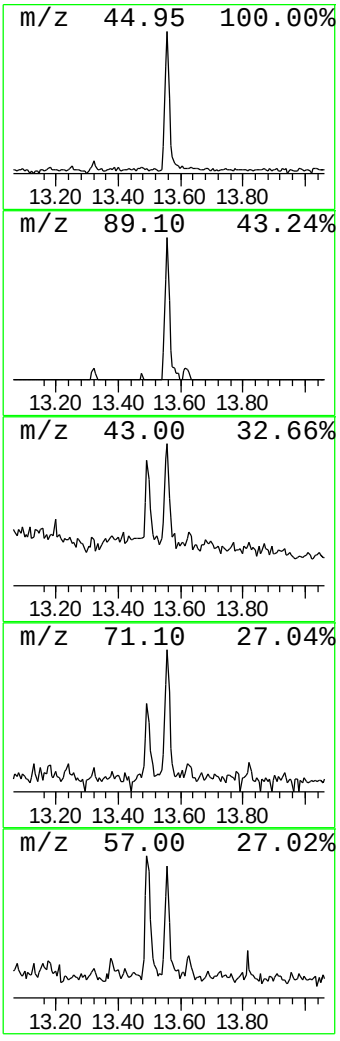
****

Peak Number 7 3,6,9,12-Tetraoxahexadecan-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	2.52 ng	104824	Chrysene-d12	13.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	80
2	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	72
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	64
4	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	64
5	Hexaethylene glycol	282	C12H26O7	002615-15-8	59





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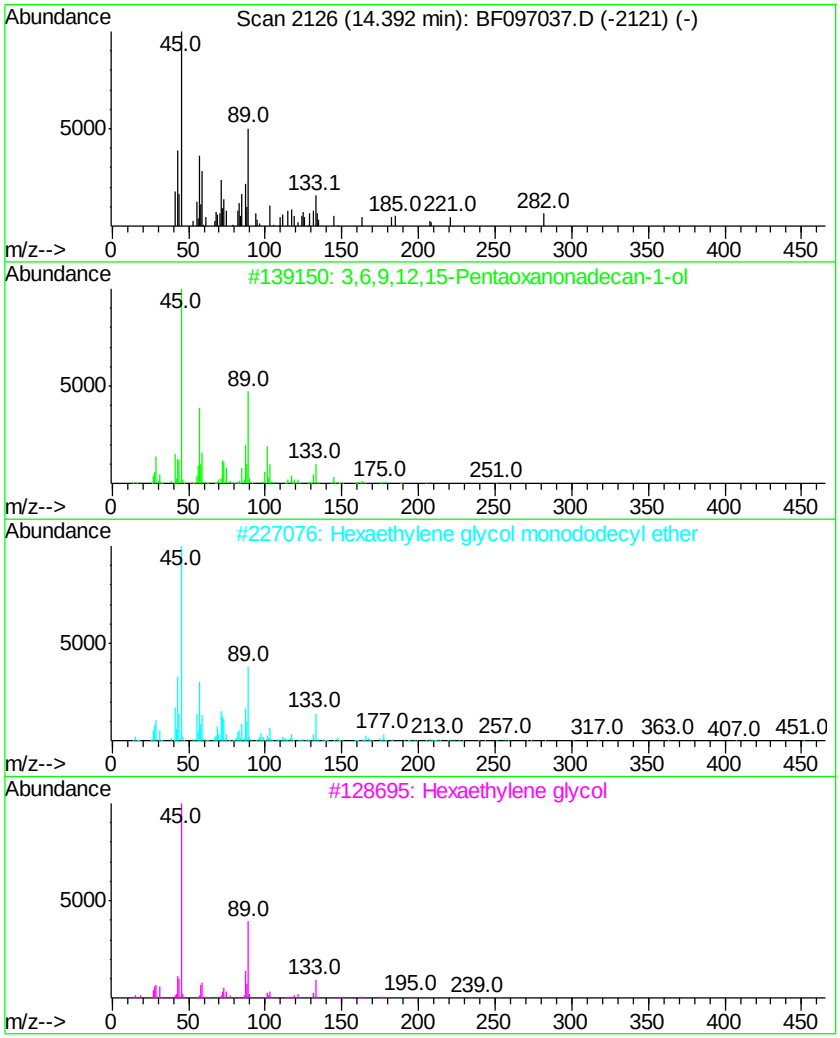
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

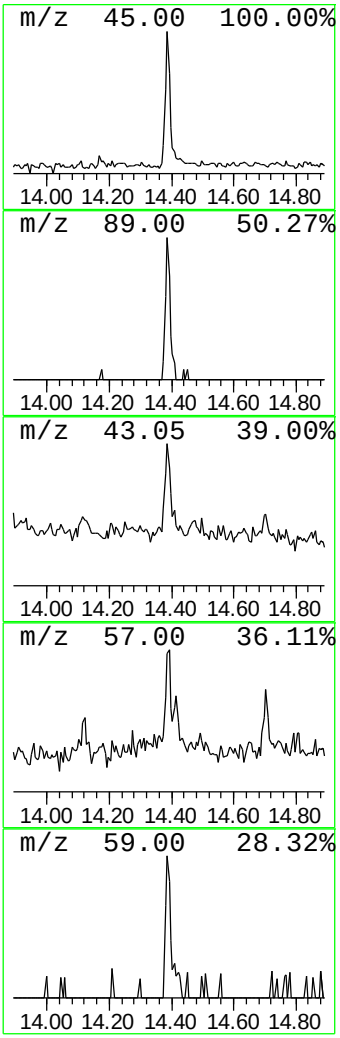
****

Peak Number 8 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	2.67 ng	69248	Perylene-d12	14.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	91
2	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	78
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	72
4	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	72
5	Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	72





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.63	2.6	ng	95500	1	6.50	722072	20.0
unknown6.27	6.27	60.9	ng	2196870	1	6.50	722072	20.0
Methoxyacetic aci...	10.40	2.1	ng	96152	4	11.00	919003	20.0
n-Hexadecanoic acid	11.56	2.0	ng	93940	4	11.00	919003	20.0
Pentaethylene glycol	11.59	3.1	ng	142724	4	11.00	919003	20.0
3,6,9,12-Tetraoxa...	13.56	2.5	ng	104824	5	13.62	830456	20.0
3,6,9,12,15-Penta...	14.39	2.7	ng	69248	6	14.97	519365	20.0