LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022819\
Data File : BG039674.D
Acq On : 1 Mar 2019 00:11
Operator : JU/SJ
Sample : K1650-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(24-25)

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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	3.217	17	22	31	rBV	95818	183975	6.33%	0.967%
2	3.294	31	35	45	rVB	48497	70539	2.43%	0.371%
3	5.708	439	446	456	rBV	838994	1343412	46.20%	7.058%
4	7.312	709	719	729	rBV	893808	1601353	55.08%	8.413%
5	7.694	775	784	792	rBV	823662	1419839	48.83%	7.460%
6	8.164	857	864	874	rVB	183017	314920	10.83%	1.655%
7	8.487	912	919	931	rVB	576591	999118	34.36%	5.249%
8	9.338	1056	1064	1073	rBV	512867	905244	31.13%	4.756%
9	10.983	1334	1344	1356	rBV	264763	477580	16.43%	2.509%
10	13.409	1749	1757	1765	rBV	1334920	2105659	72.42%	11.063%
11	14.226	1891	1896	1902	rBV	62299	93394	3.21%	0.491%
12	14.790	1981	1992	2003	rBV2	442586	723713	24.89%	3.802%
13	16.276	2238	2245	2258	rBV	1144115	1833523	63.06%	9.633%
14	17.533	2451	2459	2469	rBV2	592323	928641	31.94%	4.879%
15	18.385	2595	2604	2610	rBV3	58412	102427	3.52%	0.538%
16	20.124	2894	2900	2906	rBV	2265231	2907524	100.00%	15.276%
17	21.410	3113	3119	3127	rBV2	108217	190837	6.56%	1.003%
18	21.822	3181	3189	3199	rBV2	576672	1013608	34.86%	5.325%
19	21.968	3209	3214	3223	rVB2	40383	64772	2.23%	0.340%
20	22.597	3316	3321	3327	rBV	56858	93487	3.22%	0.491%
21	23.314	3437	3443	3450	rBV2	74299	142312	4.89%	0.748%
22	24.154	3579	3586	3594	rVB2	71179	160672	5.53%	0.844%
23	25.199	3741	3764	3775	rBV	314798	1144214	39.35%	6.012%
24	26.327	3949	3956	3972	rVB4	46111	141707	4.87%	0.745%
25	27.749	4190	4198	4208	rVB6	21709	70795	2.43%	0.372%

Sum of corrected areas: 19033265

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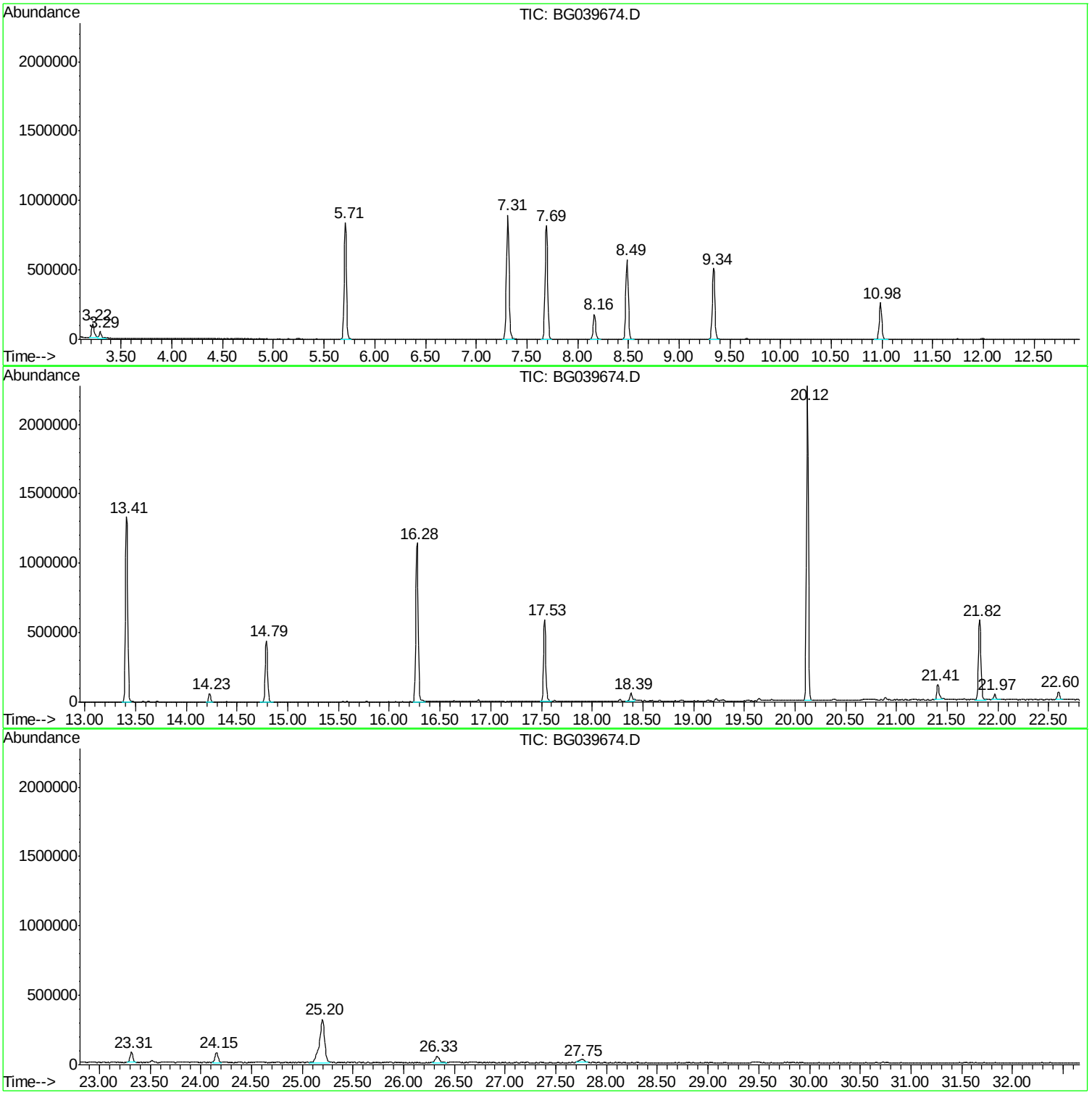
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1(24-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022819\
Data File : BG039674.D
Acq On : 1 Mar 2019 00:11
Operator : JU/SJ
Sample : K1650-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(24-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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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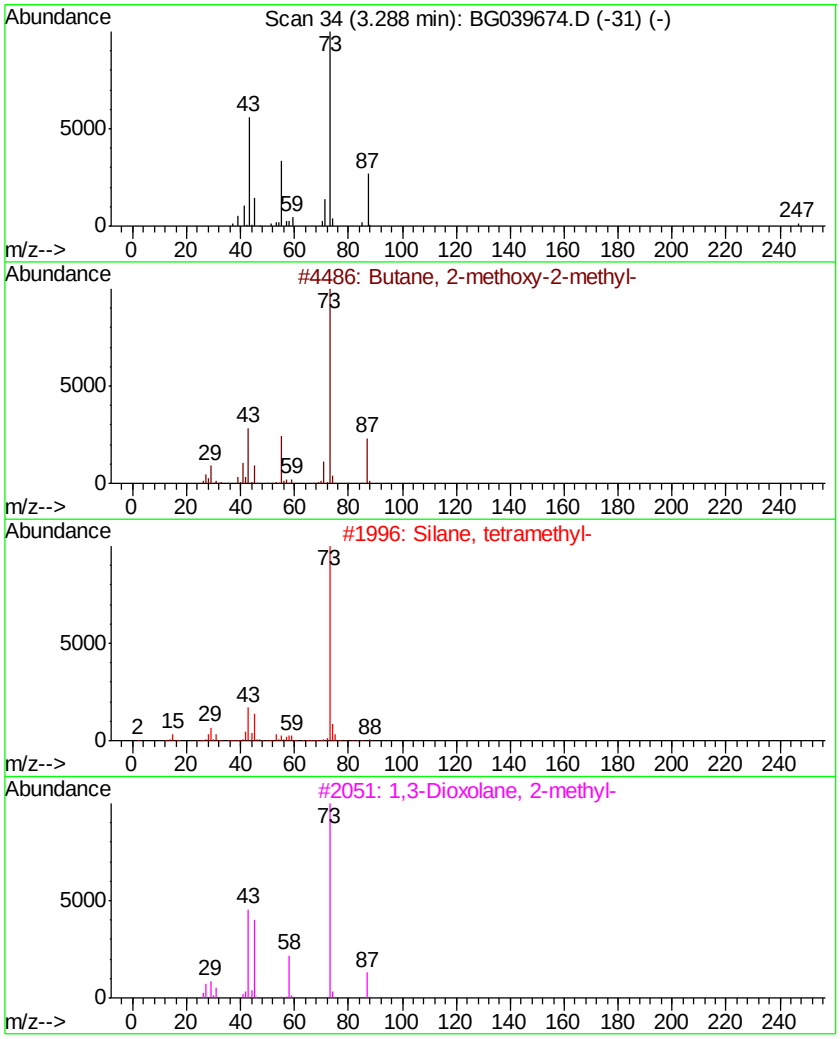
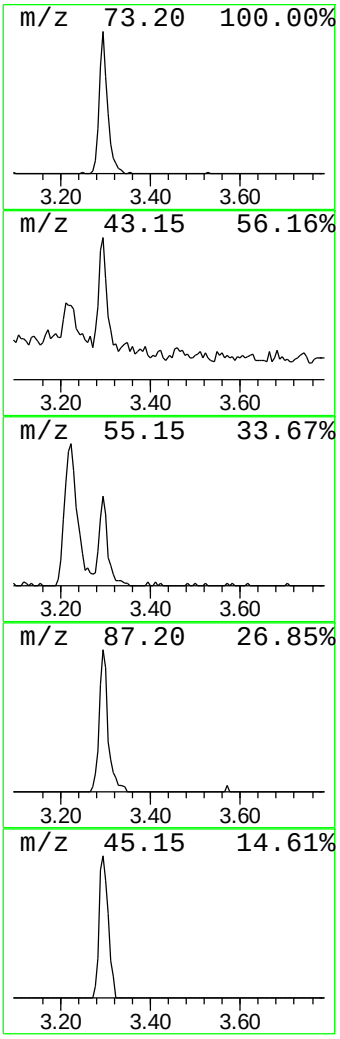
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	4.48 ng	70539	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	27
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





Library Search Compound Report

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Data File : BG039674.D
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Operator : JU/SJ
Sample : K1650-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(24-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

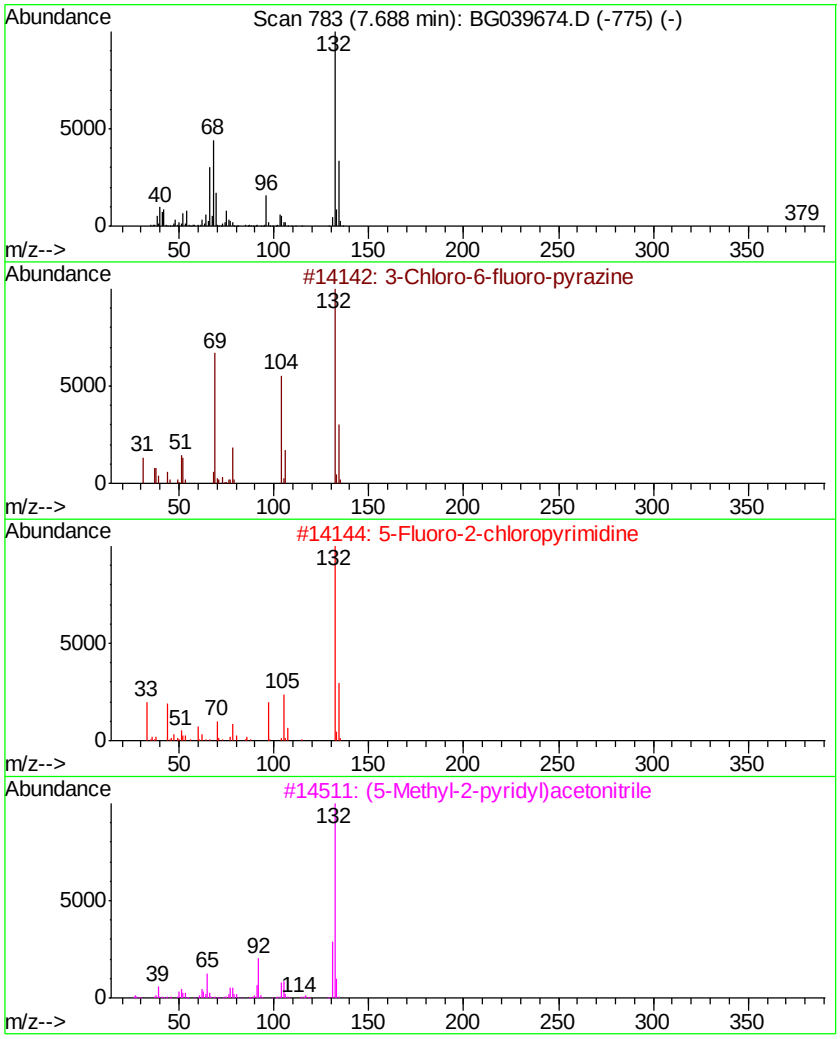
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

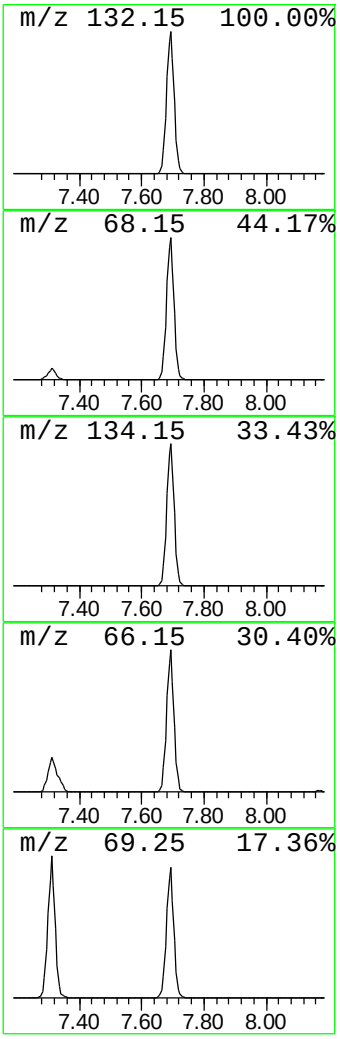
****

Peak Number 3 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	90.17 ng	1419840	1,4-Dichlorobenzene-d4	8.16

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	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





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Data File : BG039674.D
Acq On : 1 Mar 2019 00:11
Operator : JU/SJ
Sample : K1650-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(24-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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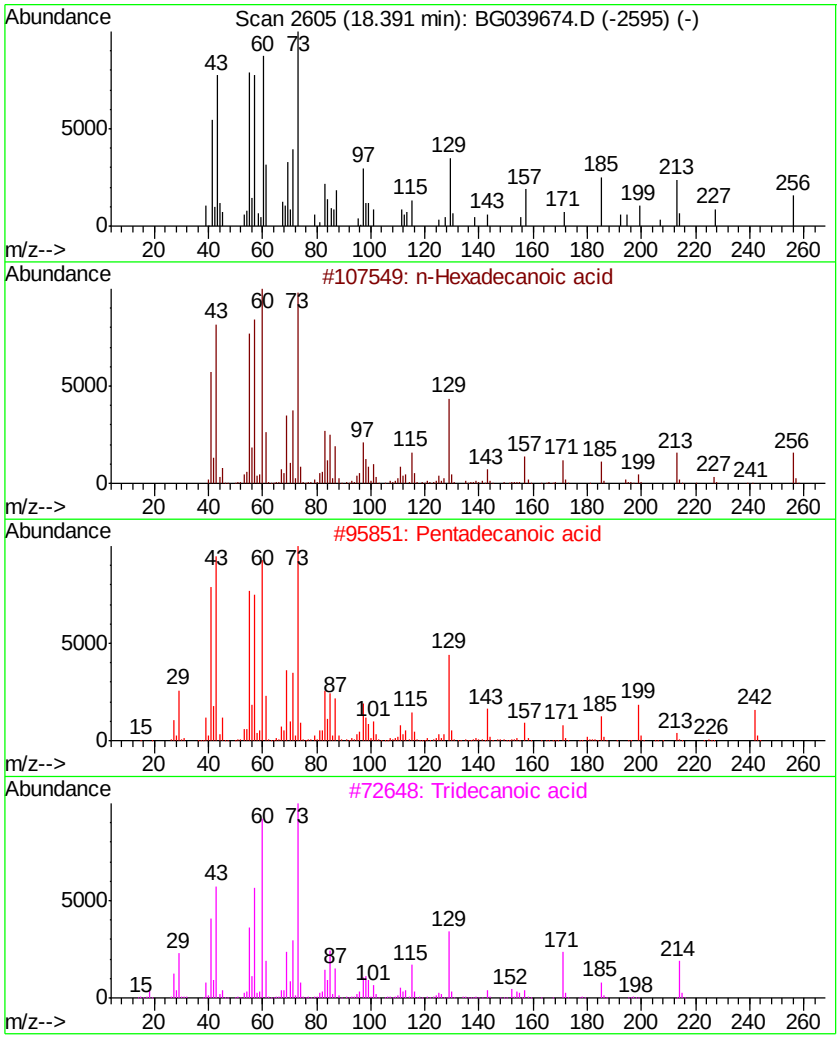
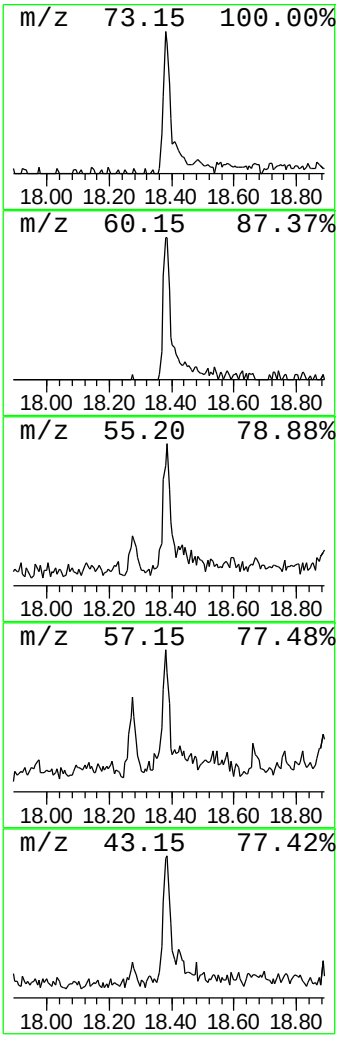
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.21 ng	102427	Phenanthrene-d10	17.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Library Search Compound Report

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Data File : BG039674.D
Acq On : 1 Mar 2019 00:11
Operator : JU/SJ
Sample : K1650-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(24-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

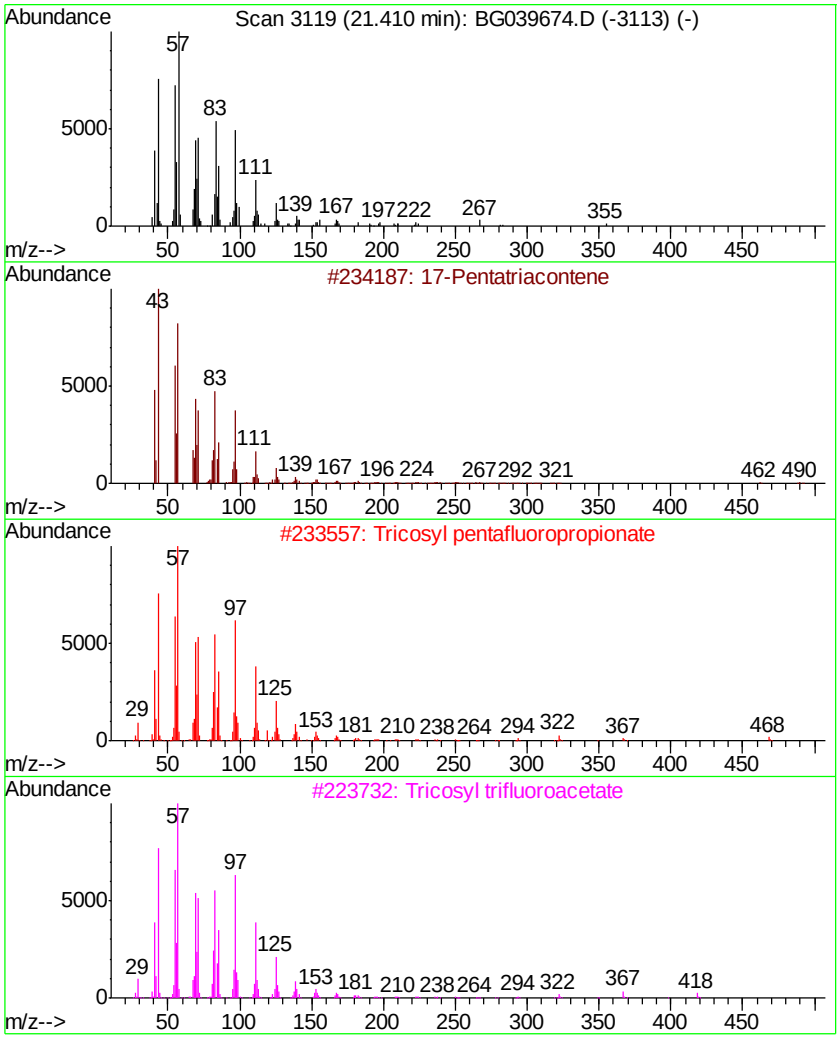
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

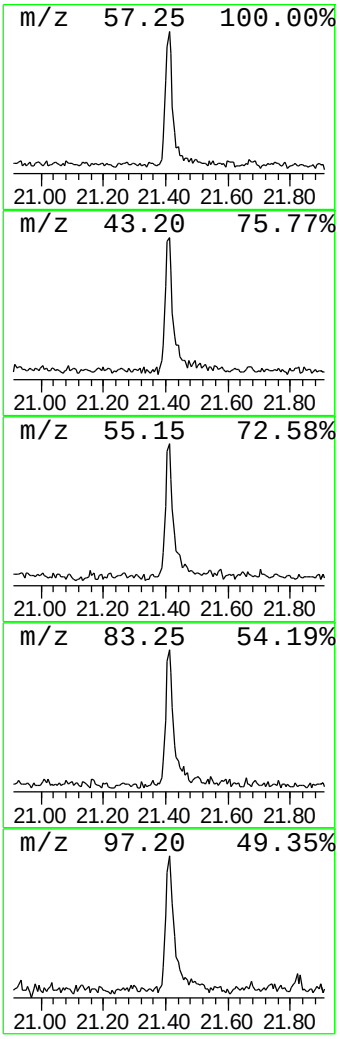
****

Peak Number 6 17-Pentatriacontene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	3.77 ng	190837	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91





Library Search Compound Report

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Operator : JU/SJ
Sample : K1650-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(24-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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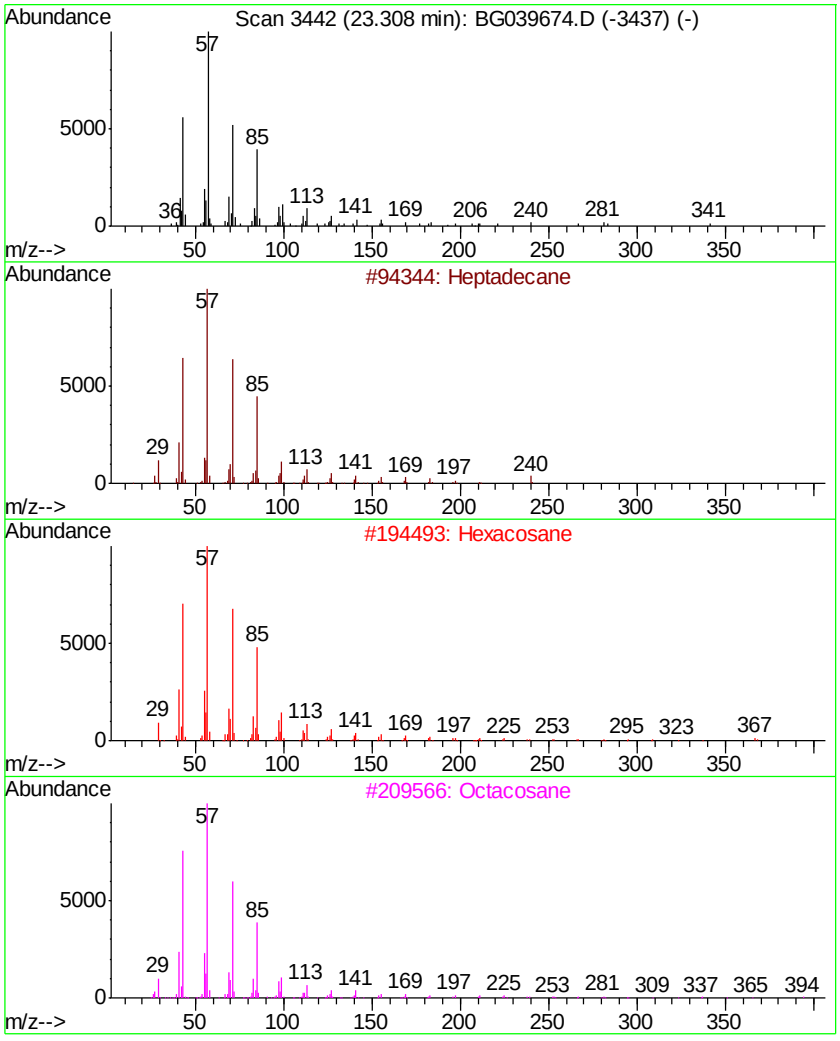
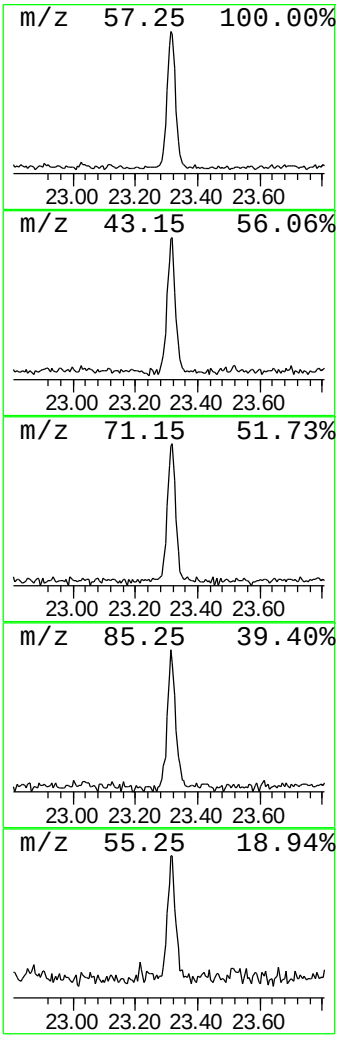
****

Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	2.81 ng	142312	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Octacosane	394	C28H58	000630-02-4	86
4	Heneicosane	296	C21H44	000629-94-7	83
5	Tetracosane	338	C24H50	000646-31-1	83





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Sample : K1650-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(24-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

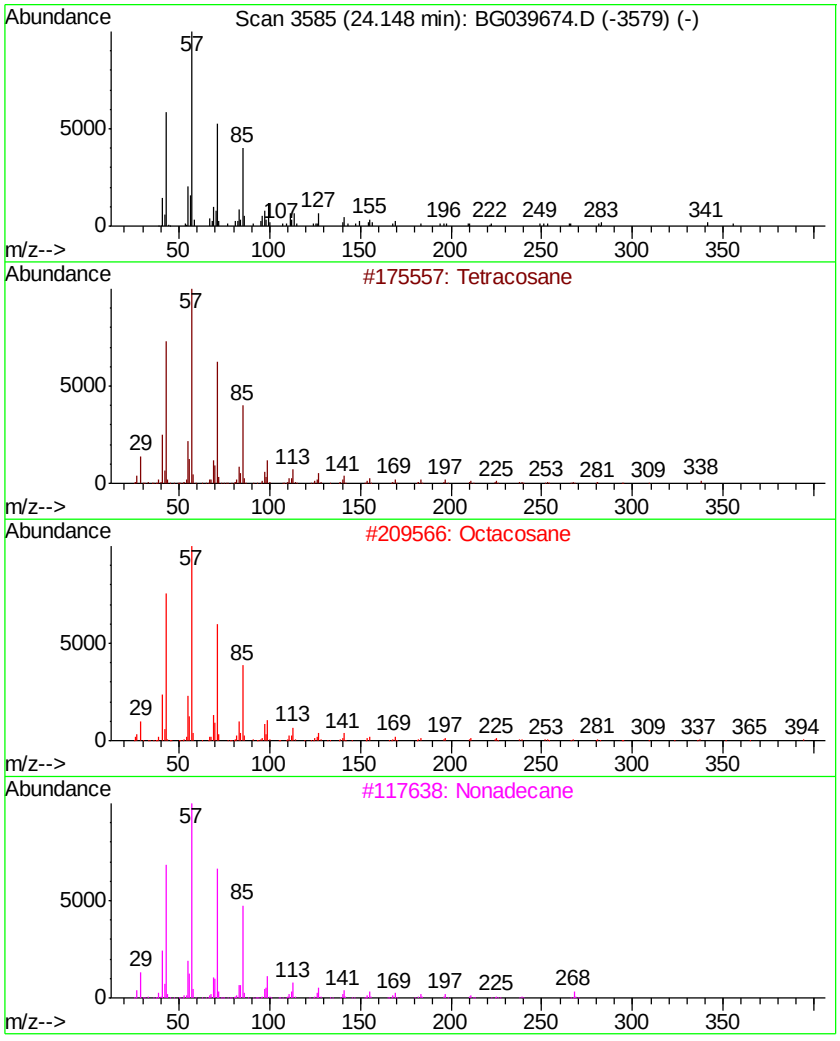
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

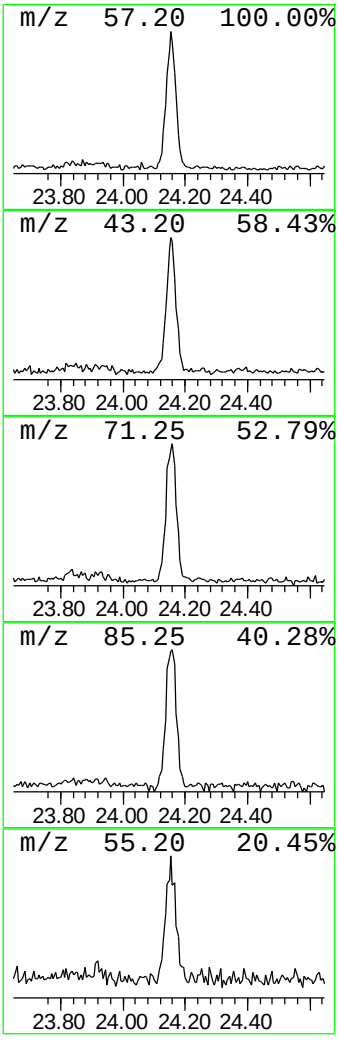
****

Peak Number 8 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.15	2.81 ng	160672	Perylene-d12	25.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Nonadecane	268	C19H40	000629-92-5	87
4	Pentacosane	352	C25H52	000629-99-2	87
5	Docosane	310	C22H46	000629-97-0	87





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Instrument : BNA_G
ClientSampleId : B-1(24-25)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

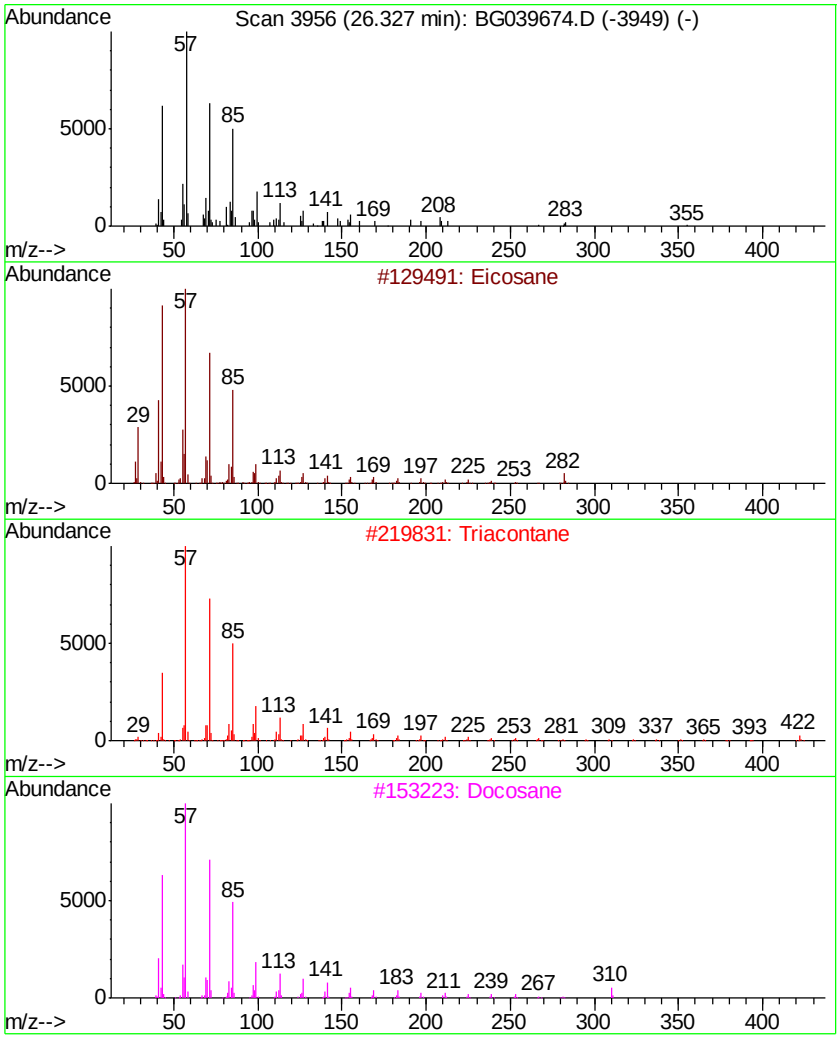
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

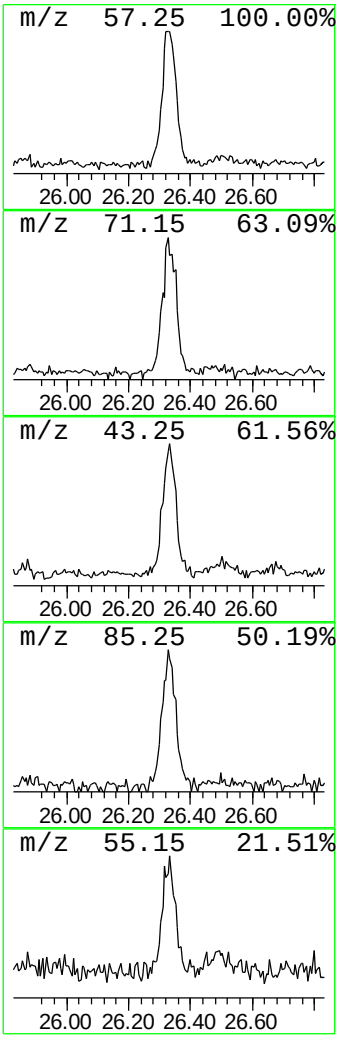
****

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.33	2.48 ng	141707	Perylene-d12	25.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Triacontane	422	C30H62	000638-68-6	87
3	Docosane	310	C22H46	000629-97-0	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Hentriacontane	437	C31H64	000630-04-6	86





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.29	4.5	ng	70539	1	8.16	314920	20.0
unknown7.69	7.69	90.2	ng	1419840	1	8.16	314920	20.0
n-Hexadecanoic acid	18.39	2.2	ng	102427	4	17.53	928641	20.0
17-Pentatriacontene	21.41	3.8	ng	190837	5	21.82	1013610	20.0
Heptadecane	23.31	2.8	ng	142312	5	21.82	1013610	20.0
Tetracosane	24.15	2.8	ng	160672	6	25.20	1144210	20.0
Eicosane	26.33	2.5	ng	141707	6	25.20	1144210	20.0