LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029267.D
Acq On : 30 Mar 2021 05:00
Operator : CG/JU
Sample : M1826-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR200035

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_M\Methods\8270-BM032621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029267.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.016	17	22	26	rBV	462567	554145	9.79%	1.436%
2	3.058	26	29	41	rVB	98443	129220	2.28%	0.335%
3	4.904	338	343	353	rBV	175954	254134	4.49%	0.659%
4	5.363	414	421	433	rBV	1880998	2803809	49.53%	7.268%
5	6.934	679	688	702	rBV	1934243	3044735	53.78%	7.892%
6	7.757	820	828	836	rBV	582393	901677	15.93%	2.337%
7	8.904	1015	1023	1034	rBV	1169171	1986049	35.08%	5.148%
8	10.539	1293	1301	1308	rBV	717281	1209134	21.36%	3.134%
9	13.004	1713	1720	1730	rBV	2748369	3921848	69.28%	10.166%
10	13.839	1856	1862	1871	rVB	79008	130225	2.30%	0.338%
11	14.216	1919	1926	1935	rVB3	25830	66552	1.18%	0.173%
12	14.380	1947	1954	1961	rBV	1015760	1527327	26.98%	3.959%
13	15.868	2200	2207	2216	rBV	1992167	2814049	49.71%	7.294%
14	16.527	2313	2319	2328	rBV5	36112	71798	1.27%	0.186%
15	17.121	2413	2420	2424	rBV	1196822	1765851	31.19%	4.577%
16	17.162	2424	2427	2432	rVB	105416	147751	2.61%	0.383%
17	17.504	2480	2485	2491	rBV3	25902	65155	1.15%	0.169%
18	18.021	2567	2573	2582	rBV	689657	1030232	18.20%	2.670%
19	18.951	2728	2731	2737	rBV2	42893	59538	1.05%	0.154%
20	19.174	2763	2769	2783	rBV2	535394	1361169	24.04%	3.528%
21	19.298	2786	2790	2799	rVB2	448866	648483	11.45%	1.681%
22	19.533	2826	2830	2837	rVB	278579	405302	7.16%	1.051%
23	19.739	2860	2865	2876	rVB	4559674	5661232	100.00%	14.674%
24	20.027	2911	2914	2917	rBV2	51553	64875	1.15%	0.168%
25	20.056	2917	2919	2923	rVB	77704	82346	1.45%	0.213%
26	21.003	3076	3080	3086	rBV	762567	913603	16.14%	2.368%
27	21.209	3111	3115	3119	rBV	566507	603194	10.65%	1.564%
28	21.286	3123	3128	3132	rBV	1655358	2236167	39.50%	5.796%
29	21.892	3227	3231	3236	rBV2	332109	443719	7.84%	1.150%
30	22.850	3391	3394	3397	rBV	264747	382232	6.75%	0.991%
31	22.892	3398	3401	3408	rVB3	393679	603434	10.66%	1.564%
32	23.527	3503	3509	3515	rVB	1109191	1970560	34.81%	5.108%
33	24.150	3611	3615	3625	rVB2	381193	719908	12.72%	1.866%

Sum of corrected areas: 38579453

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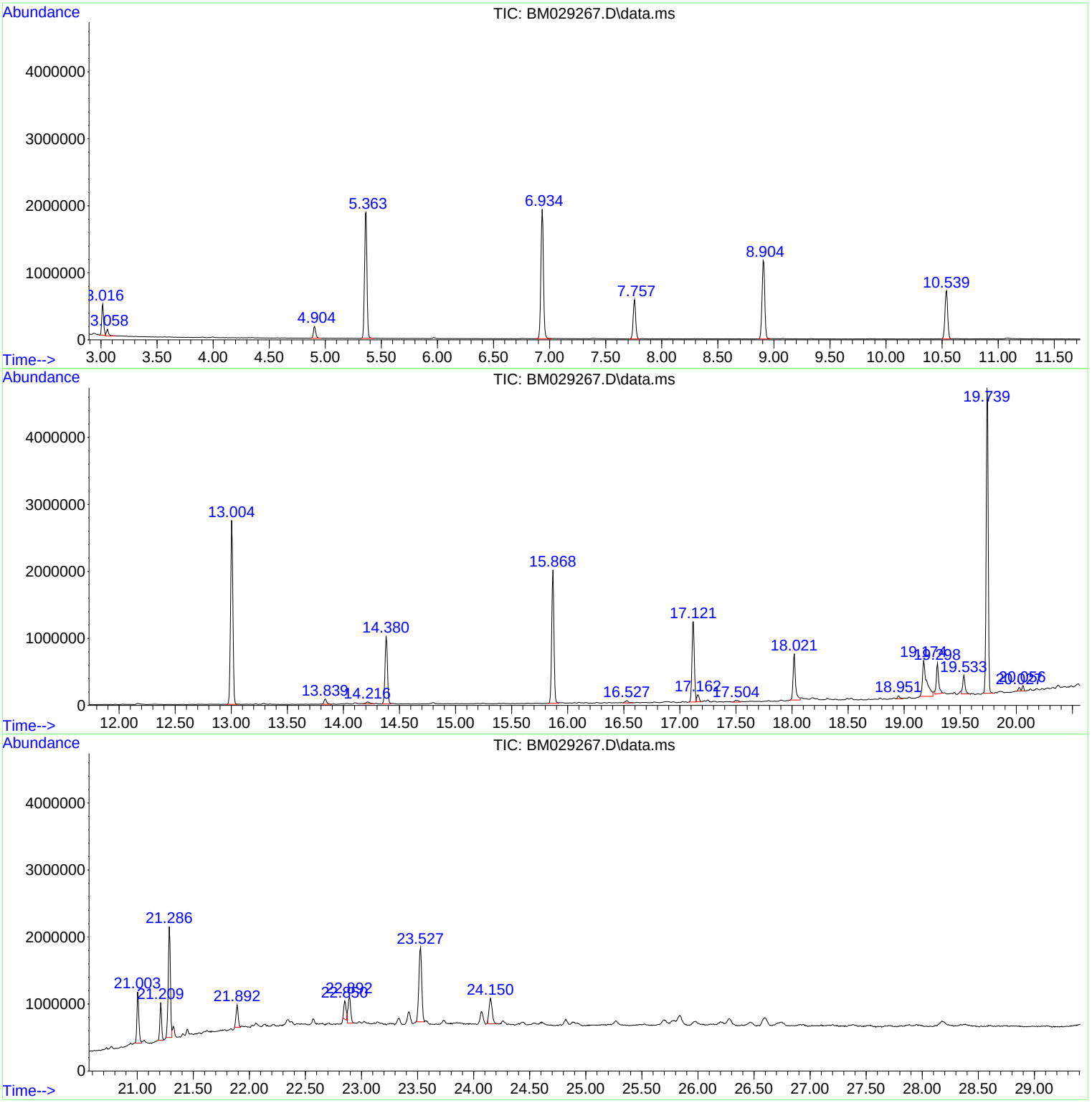
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RO-RBR200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.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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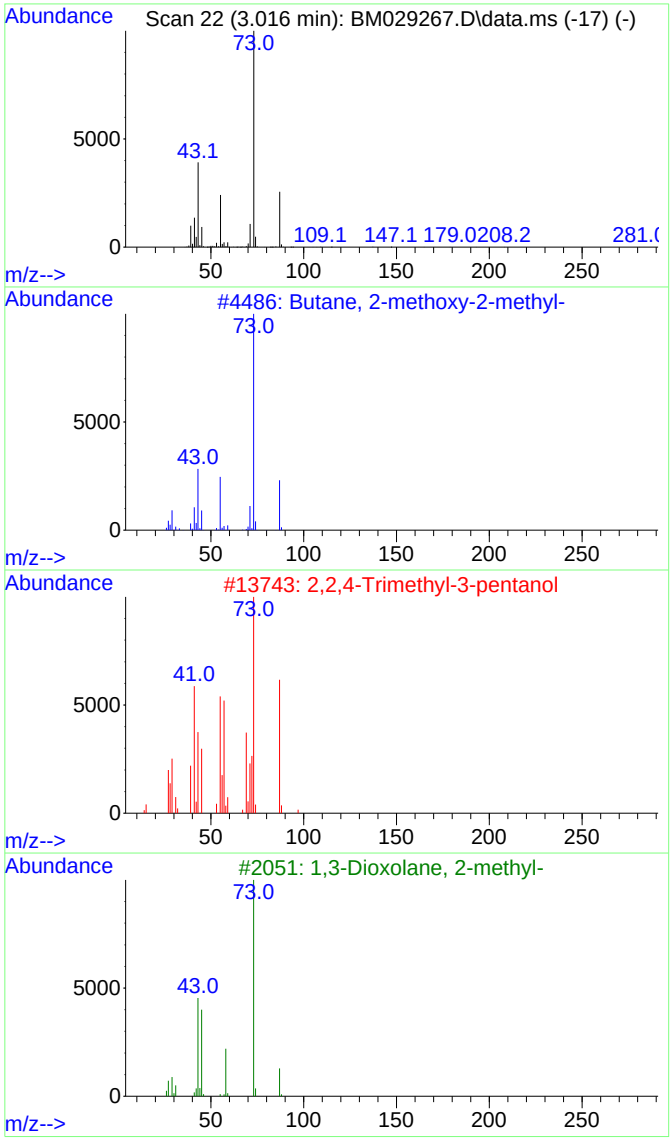
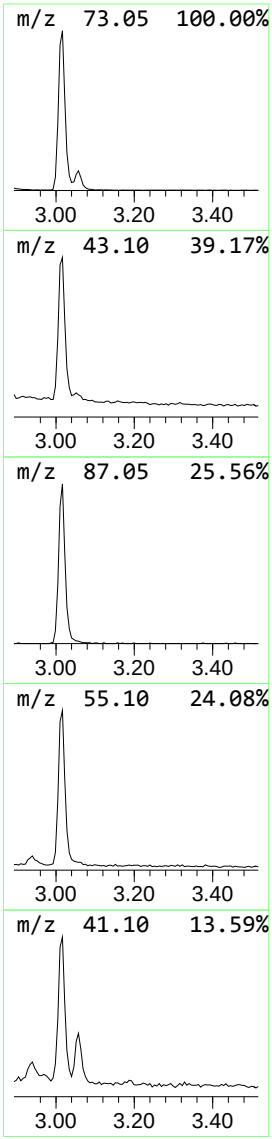
****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.016	12.29 ng	554145	1,4-Dichlorobenzene-d4	7.757

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	50
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Operator : CG/JU
Sample : M1826-01
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ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

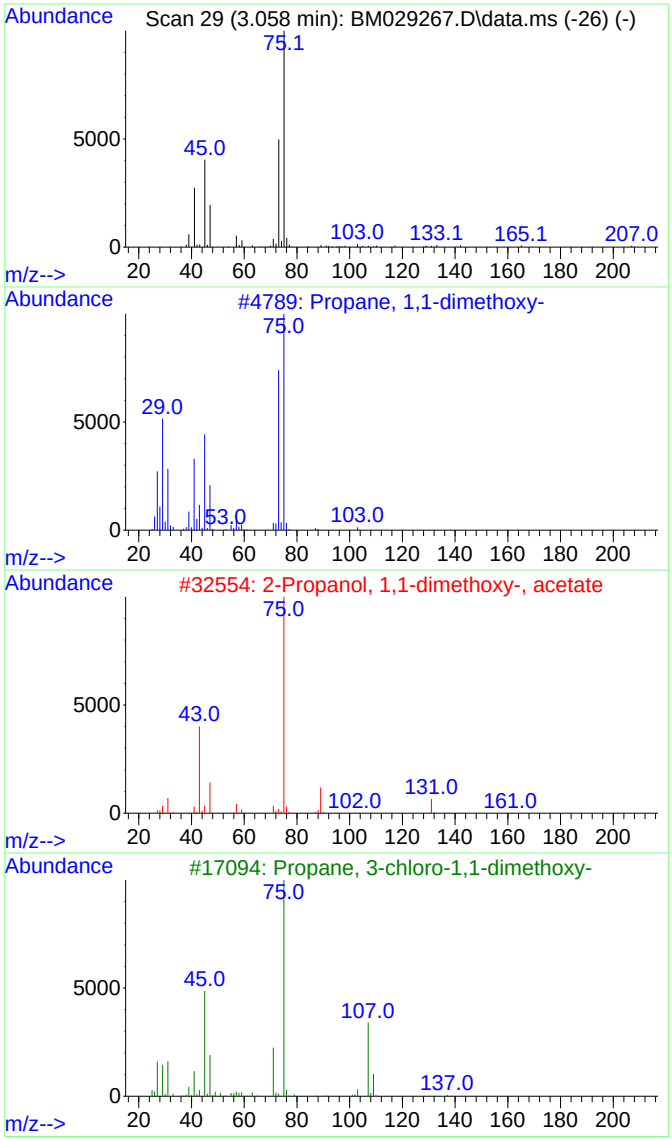
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

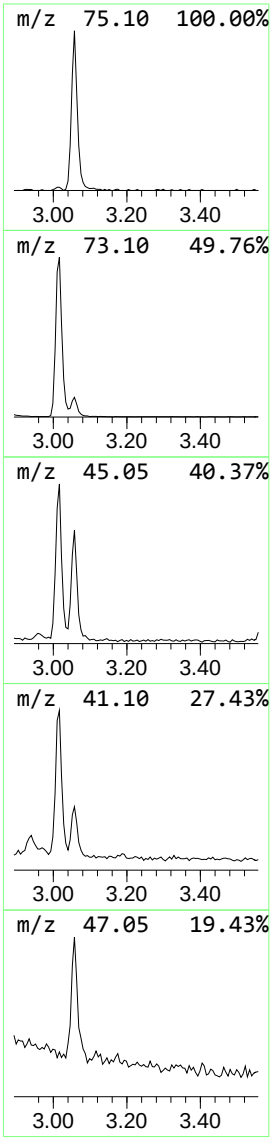
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.058	2.87 ng	129220	1,4-Dichlorobenzene-d4	7.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2	2-Propanol, 1,1-dimethoxy-, acetate	162	C7H14O4	074495-37-7	42
3	Propane, 3-chloro-1,1-dimethoxy-	138	C5H11ClO2	035502-06-8	39
4	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	38
5	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	36





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Sample : M1826-01
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Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
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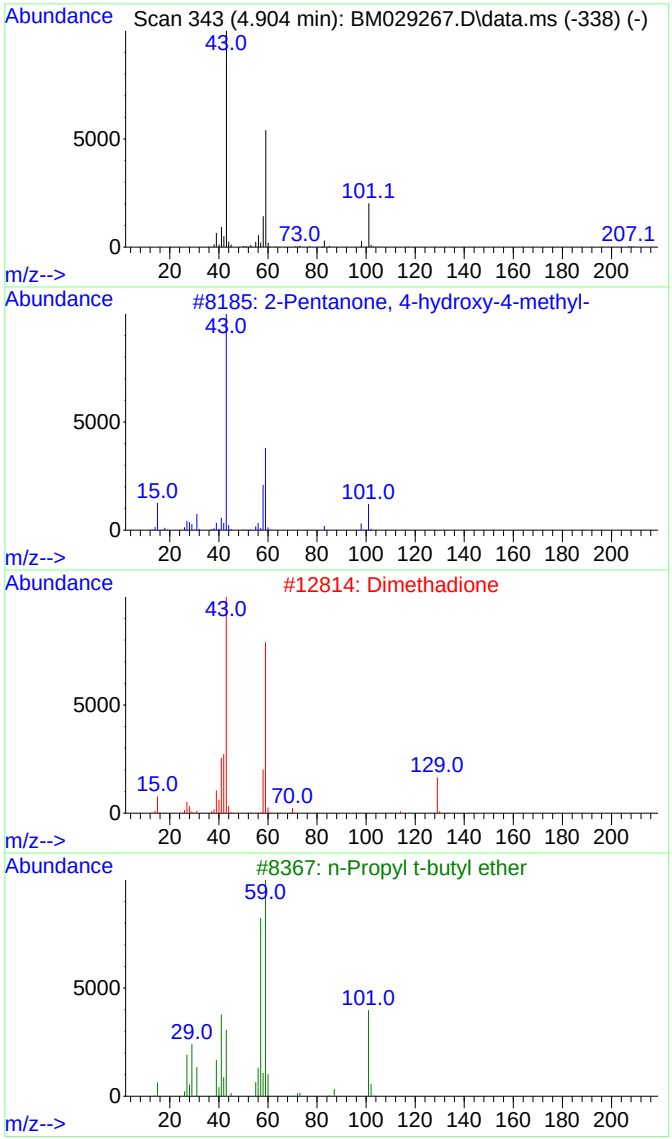
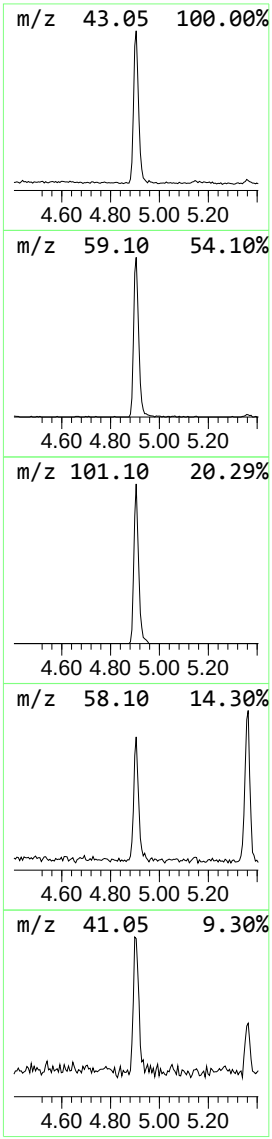
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	5.64 ng	254134	1,4-Dichlorobenzene-d4	7.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Dimethadione	129	C5H7NO3	000695-53-4	40
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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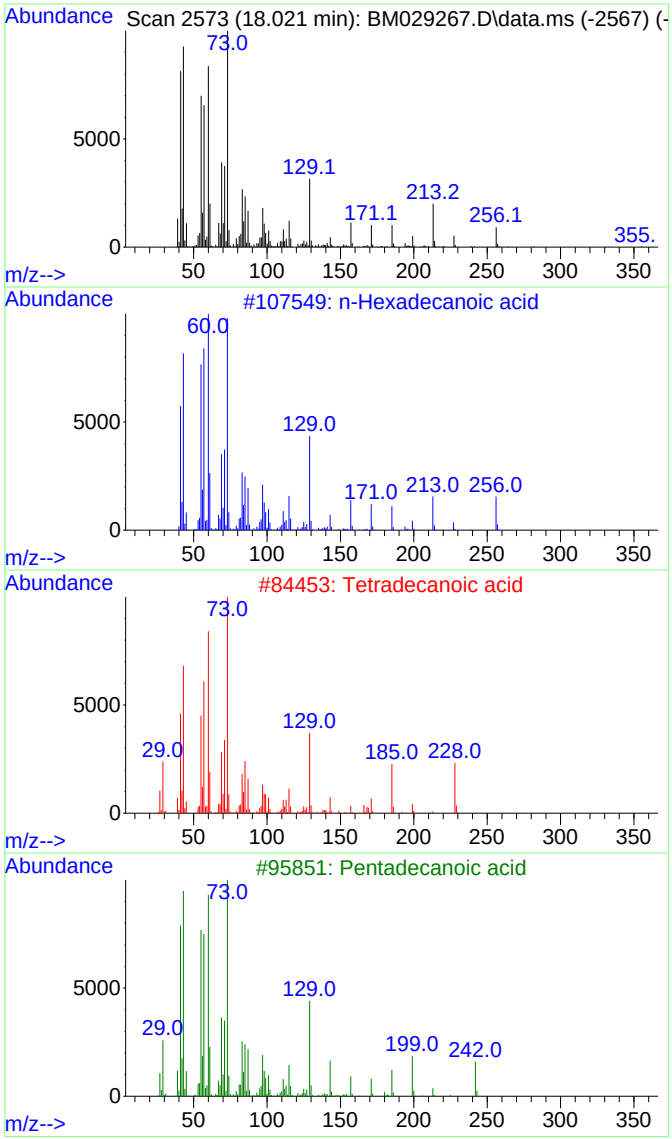
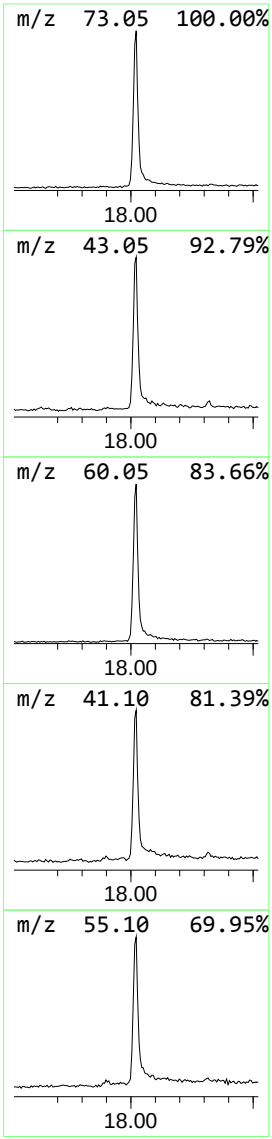
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.021	11.67 ng	1030230	Phenanthrene-d10	17.121

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Octadecanoic acid	284	C18H36O2	000057-11-4	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
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Sample : M1826-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : RO-RBR200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.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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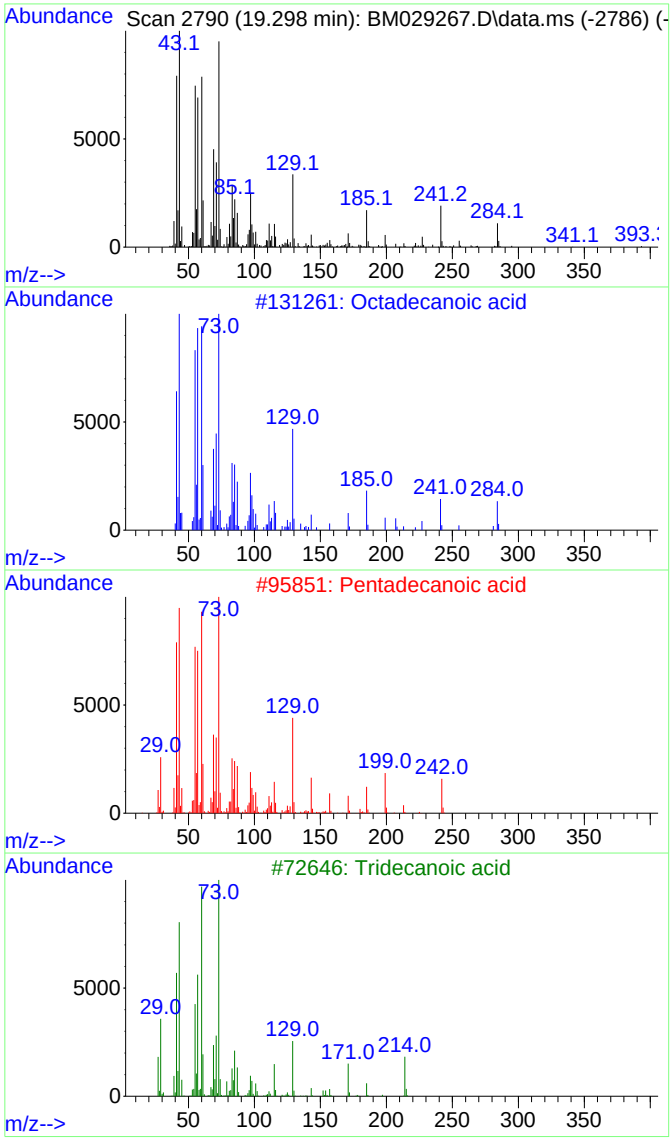
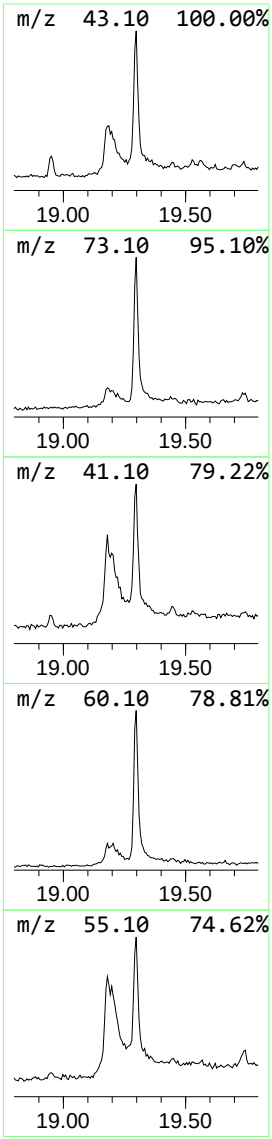
Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.298	5.80 ng	648483	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53





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Instrument :
BNA_M
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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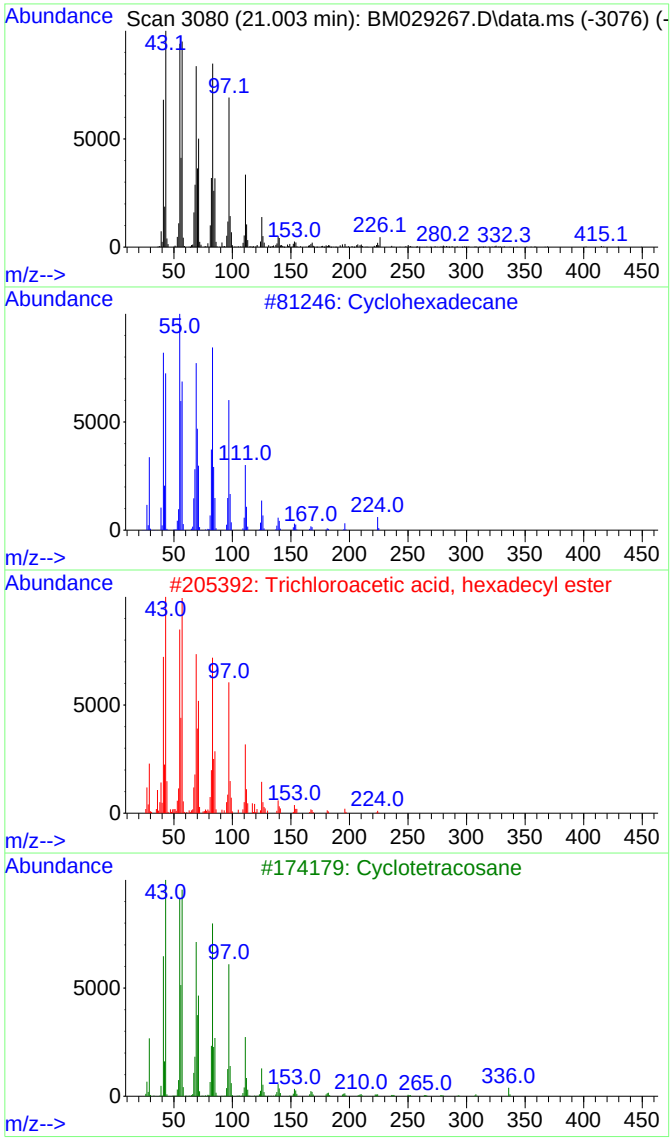
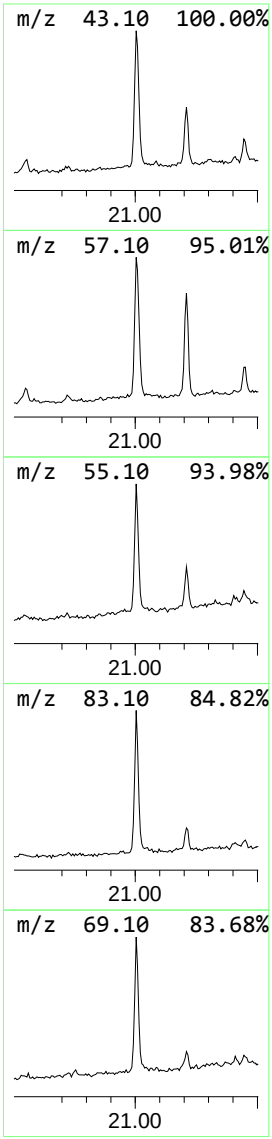
Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.003	8.17 ng	913603	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	97
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Cyclotetracosane	336	C24H48	000297-03-0	93
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





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Sample : M1826-01
Misc :
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Instrument : BNA_M
ClientSampleId : RO-RBR200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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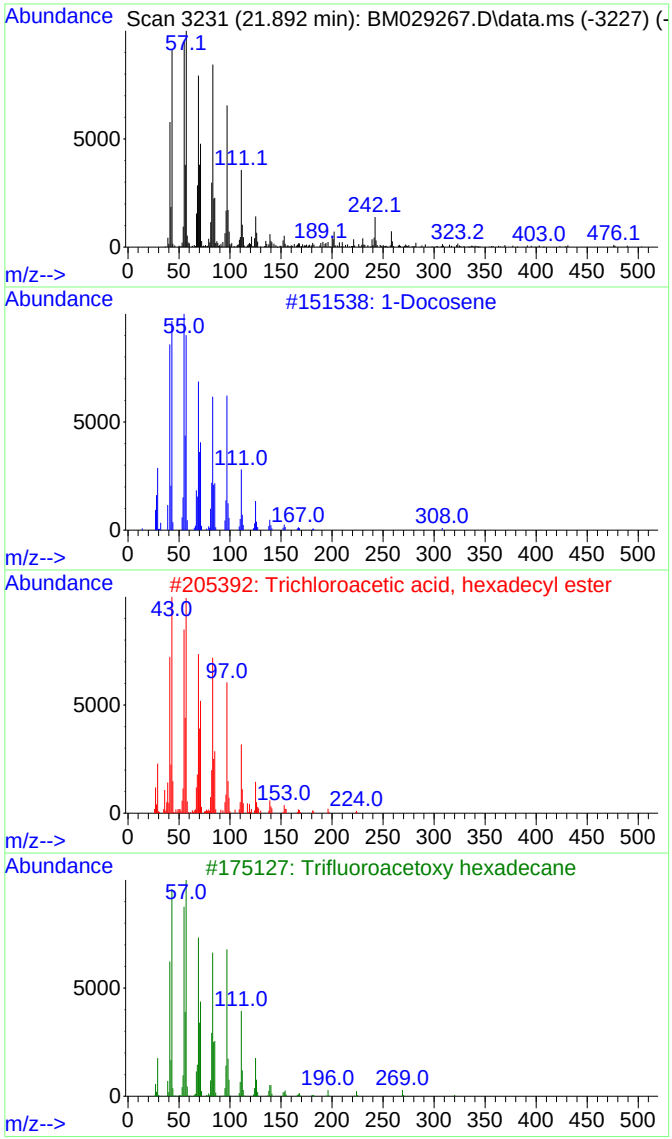
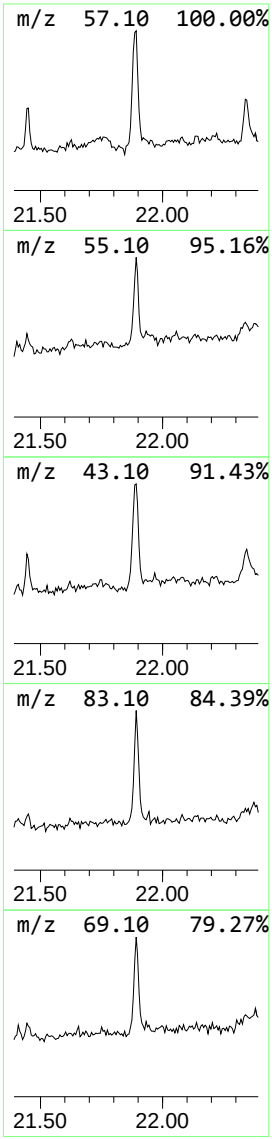
Peak Number 7 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.892	3.97 ng	443719	Chrysene-d12	21.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	97
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Cyclopentadecane	210	C15H30	000295-48-7	93
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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TIC Library : C:\DATABASE\NIST11.L
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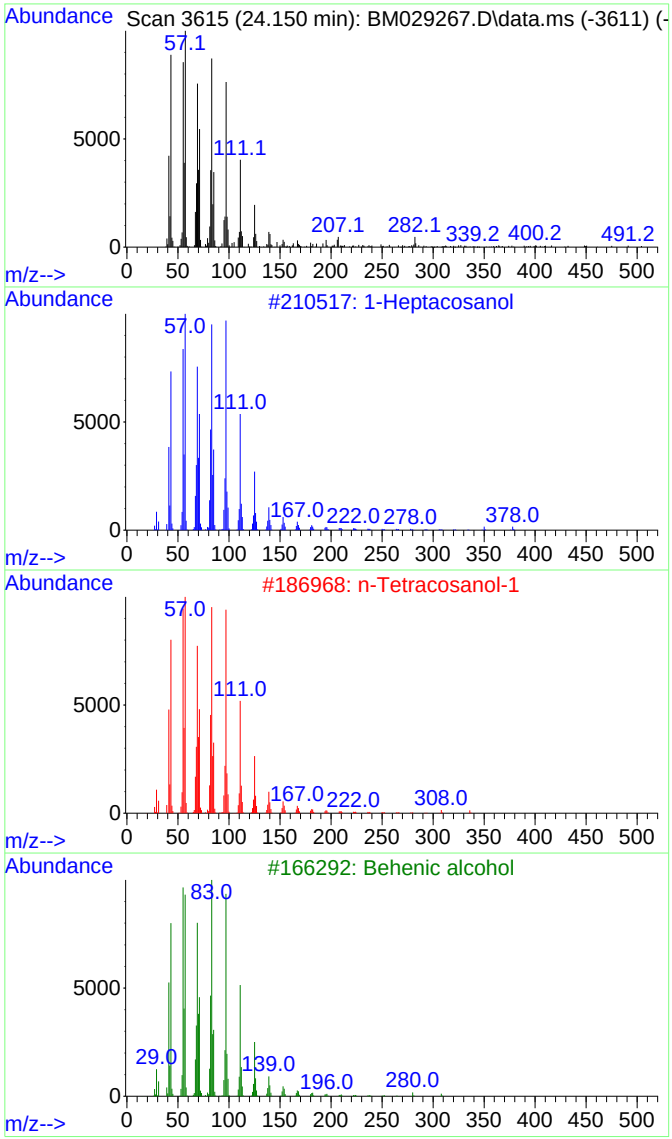
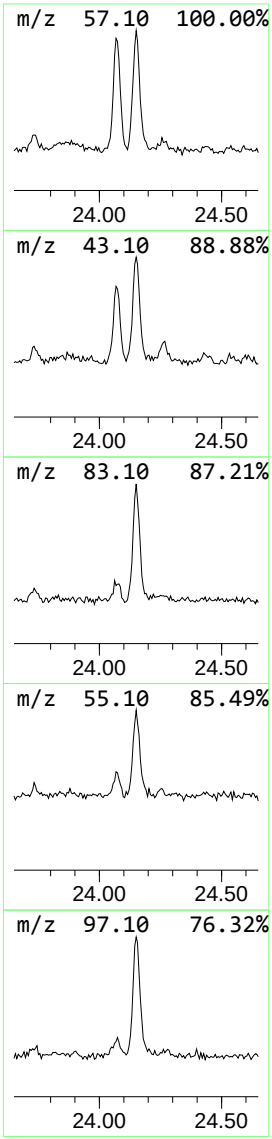
Peak Number 8 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.150	7.31 ng	719908	Perylene-d12	23.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	17-Pentatriacontene	491	C35H70	006971-40-0	87
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	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
Butane, 2-metho...	3.016	12.3	ng	554145	1	7.757	901677	20.0
Propane, 1,1-di...	3.058	2.9	ng	129220	1	7.757	901677	20.0
2-Pentanone, 4-...	4.904	5.6	ng	254134	1	7.757	901677	20.0
n-Hexadecanoic ...	18.021	11.7	ng	1030230	4	17.121	1765850	20.0
Octadecanoic acid	19.298	5.8	ng	648483	5	21.286	2236170	20.0
Cyclohexadecane	21.003	8.2	ng	913603	5	21.286	2236170	20.0
1-Docosene	21.892	4.0	ng	443719	5	21.286	2236170	20.0
1-Heptacosanol	24.150	7.3	ng	719908	6	23.527	1970560	20.0