LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023425.D
Acq On : 3 Aug 2016 14:37
Operator : UM/SJ
Sample : H4287-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-14.0-15.0

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_G\METHODS\8270-BG080116.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	2.991	21	26	41	rVB	2037297	2848234	33.32%	5.492%
2	5.182	393	399	406	rBV	496413	739356	8.65%	1.426%
3	5.658	473	480	494	rBV	1792803	2953400	34.55%	5.694%
4	7.274	746	755	771	rBV	1939824	3459005	40.46%	6.669%
5	7.644	811	818	827	rBV	1808235	3200467	37.44%	6.171%
6	8.120	892	899	908	rBV	391984	675498	7.90%	1.302%
7	8.443	944	954	964	rBV	1257275	2240678	26.21%	4.320%
8	9.294	1091	1099	1110	rBV	1182969	2127673	24.89%	4.102%
9	9.406	1112	1118	1124	rBV3	57010	101426	1.19%	0.196%
10	10.951	1373	1381	1389	rBV	568114	1034804	12.11%	1.995%
11	13.395	1789	1797	1809	rBV	3185967	5116915	59.86%	9.866%
12	14.223	1931	1938	1945	rBV	1436593	2133795	24.96%	4.114%
13	14.781	2026	2033	2043	rBV2	999432	1648080	19.28%	3.178%
14	15.604	2169	2173	2179	rVB2	75891	111876	1.31%	0.216%
15	16.279	2282	2288	2300	rBV	3278371	5059922	59.19%	9.756%
16	16.467	2316	2320	2330	rBV	100602	185476	2.17%	0.358%
17	17.272	2453	2457	2460	rBV2	66444	85811	1.00%	0.165%
18	17.542	2497	2503	2510	rBV2	1492929	2352352	27.52%	4.536%
19	17.900	2560	2564	2575	rBV2	245952	476933	5.58%	0.920%
20	18.417	2647	2652	2661	rBV	346809	565437	6.61%	1.090%
21	19.680	2862	2867	2883	rBV	346975	562028	6.57%	1.084%
22	19.827	2888	2892	2900	rVB3	142259	185284	2.17%	0.357%
23	20.150	2941	2947	2953	rBV	6211208	8548452	100.00%	16.482%
24	20.826	3055	3062	3066	rBV2	78555	139440	1.63%	0.269%
25	20.873	3066	3070	3074	rVB2	97442	112467	1.32%	0.217%
26	21.466	3167	3171	3174	rBV6	58018	89219	1.04%	0.172%
27	21.860	3231	3238	3248	rVB	1595633	2671507	31.25%	5.151%
28	25.238	3802	3813	3824	rBV	847600	2439062	28.53%	4.703%

Sum of corrected areas: 51864597

LSC Report - Integrated Chromatogram

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Data File : BG023425.D
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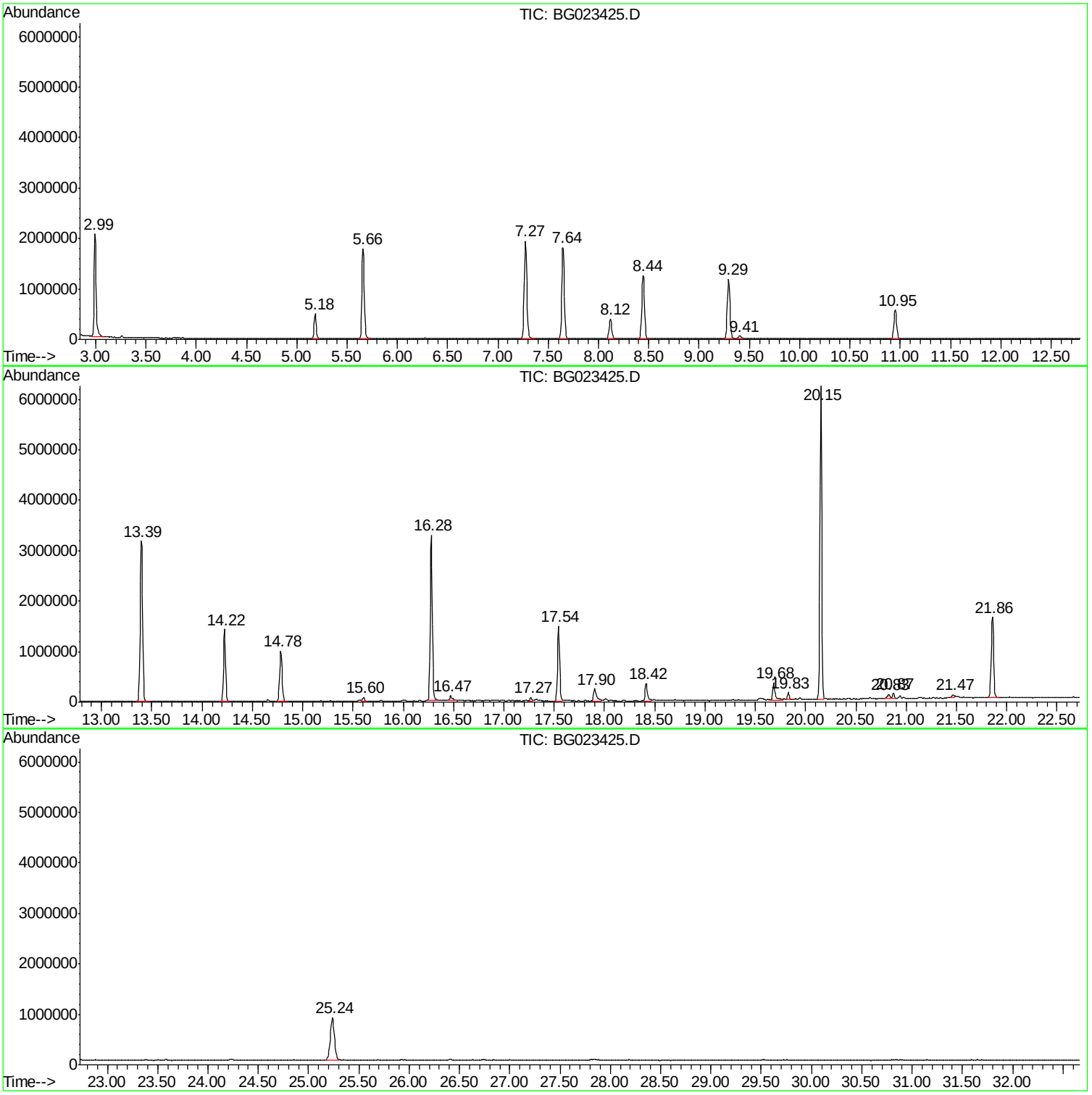
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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 G\DATA\BG080316\
Data File : BG023425.D
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Operator : UM/SJ
Sample : H4287-09
Misc :
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Instrument : BNA_G
ClientSampleId : SB-60-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

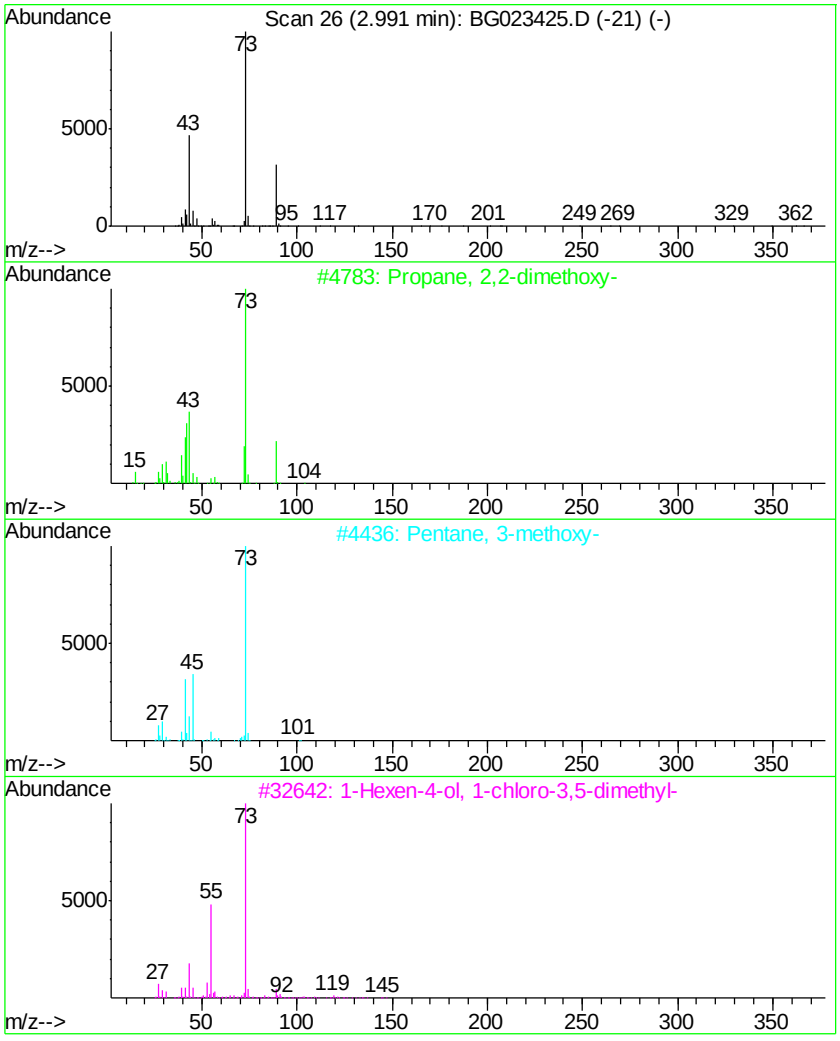
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

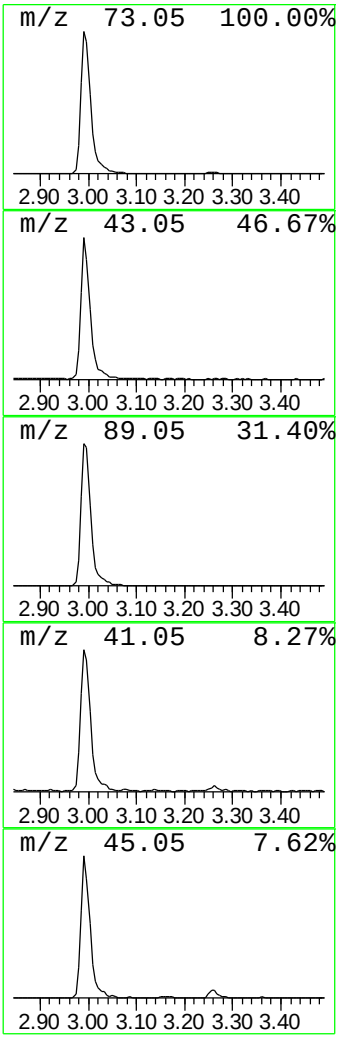
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	84.33 ng	2848230	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Data File : BG023425.D
Acq On : 3 Aug 2016 14:37
Operator : UM/SJ
Sample : H4287-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

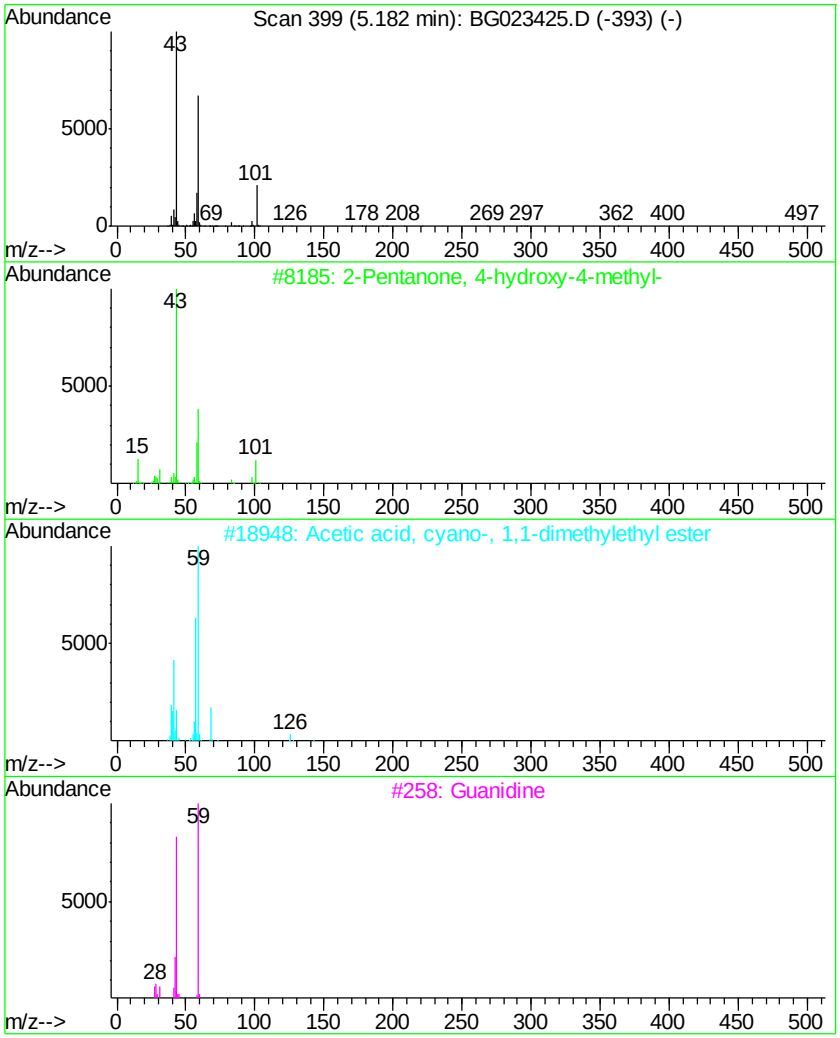
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

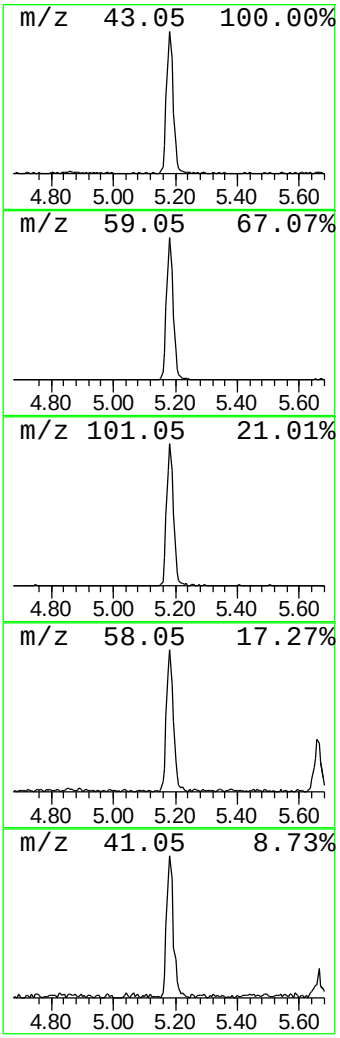
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	21.89 ng	739356	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Guanidine	59	CH5N3	000113-00-8	9
4	Acetone	58	C3H6O	000067-64-1	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023425.D
Acq On : 3 Aug 2016 14:37
Operator : UM/SJ
Sample : H4287-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

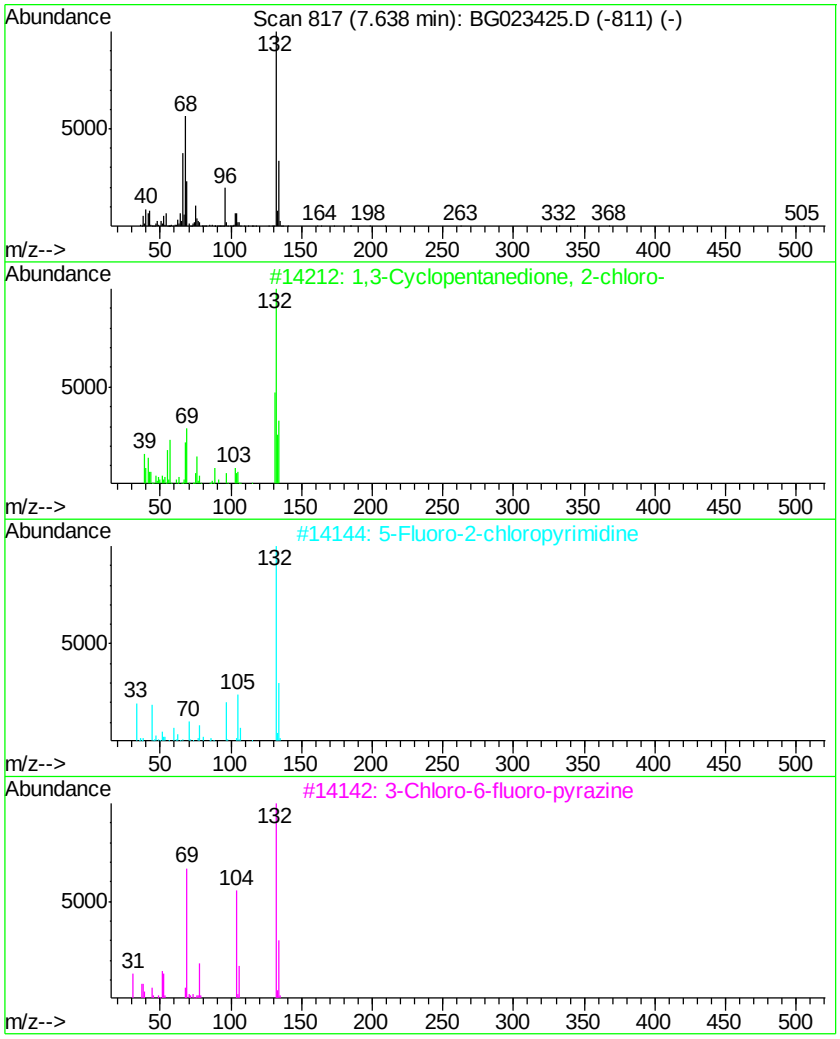
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

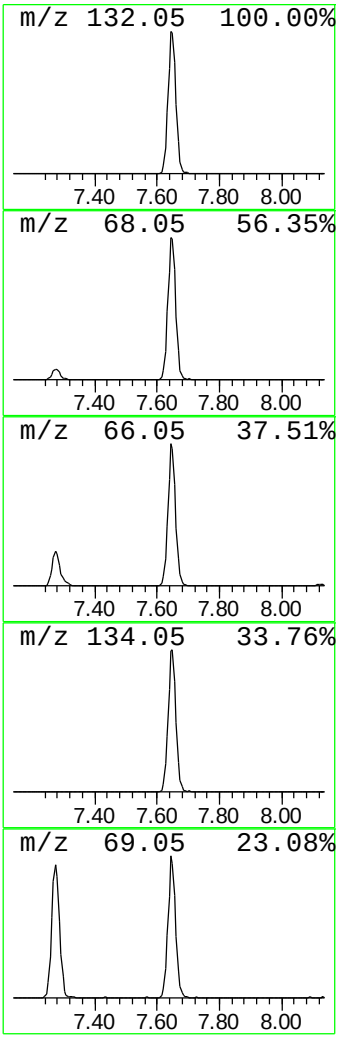
****

Peak Number 3 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	94.76 ng	3200470	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

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Operator : UM/SJ
Sample : H4287-09
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-60-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

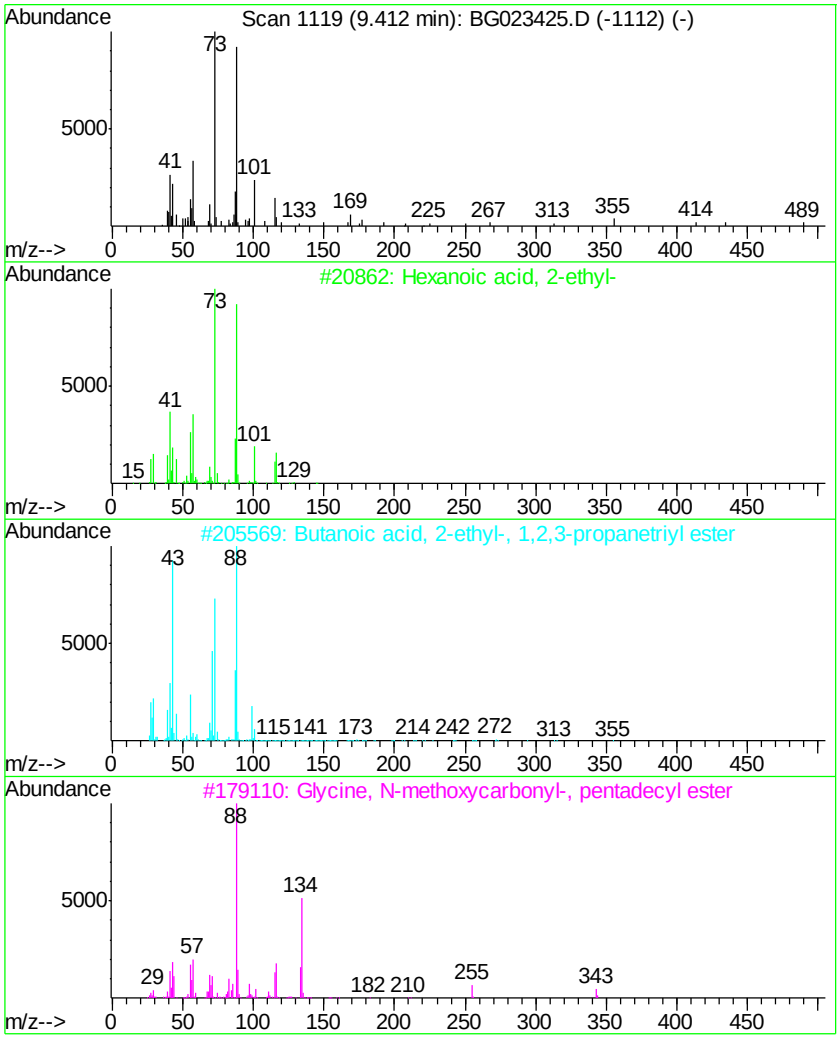
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

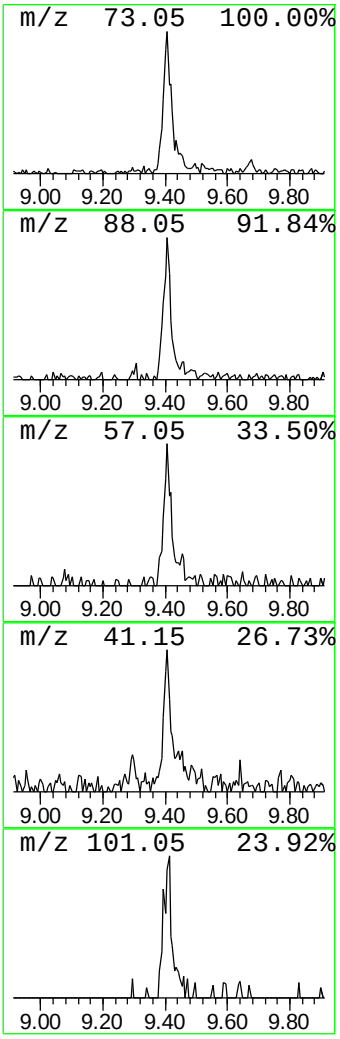
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.41	3.00 ng	101426	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	64
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3	Glycine, N-methoxycarbonyl-, pen...	343	C19H37NO4	1000313-49-5	38
4	Glycine, N-methoxycarbonyl-, hex...	357	C20H39NO4	1000313-49-6	38
5	Glycine, N-methoxycarbonyl-, hep...	371	C21H41NO4	1000313-49-7	38





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
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Sample : H4287-09
Misc :
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Instrument : BNA_G
ClientSampleId : SB-60-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

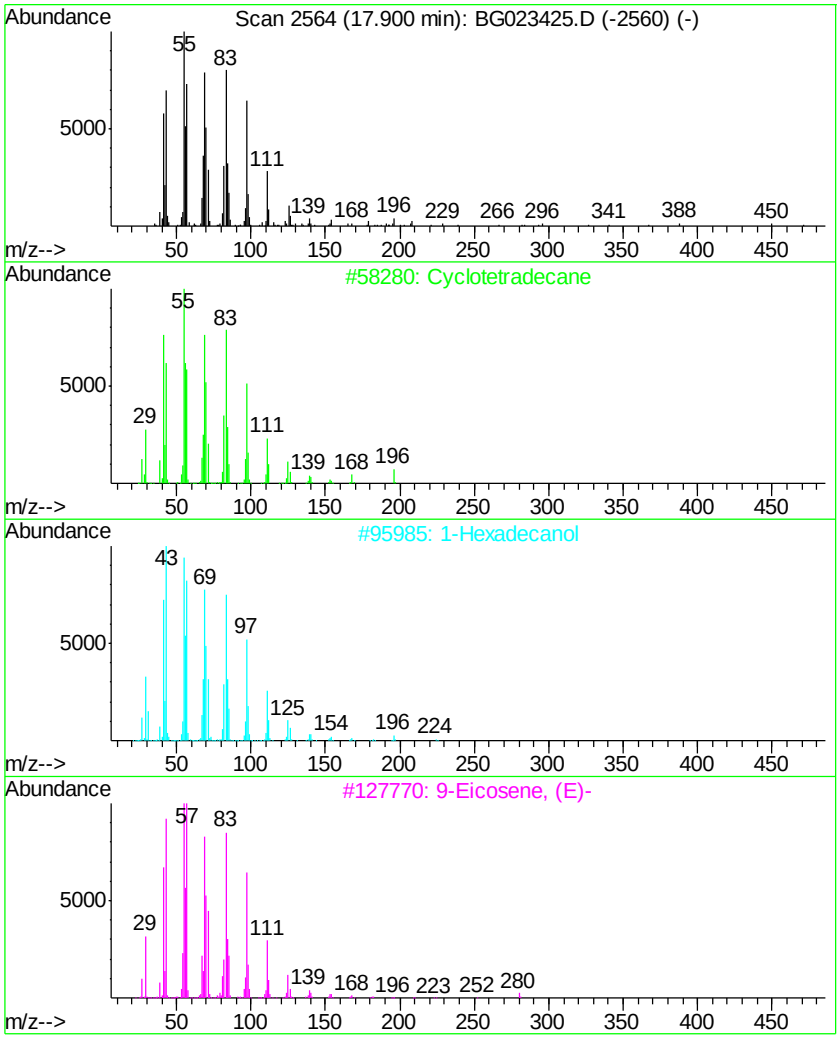
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

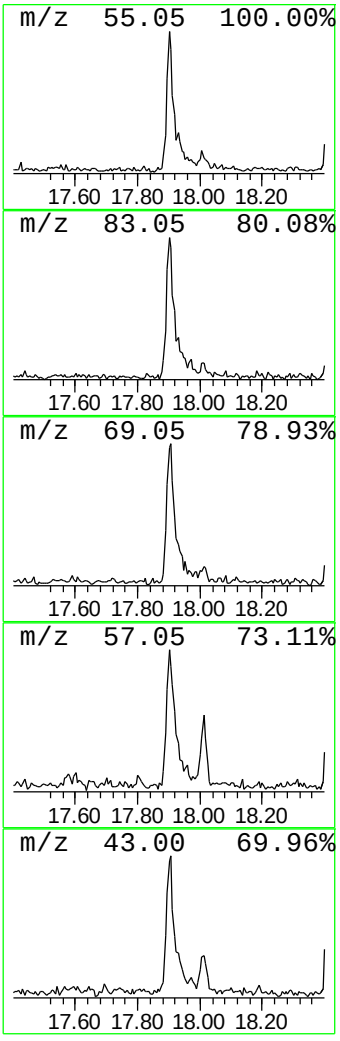
****

Peak Number 6 Cyclotetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.90	4.05 ng	476933	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	94
2	1-Hexadecanol	242	C16H34O	036653-82-4	94
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	n-Pentadecanol	228	C15H32O	000629-76-5	91
5	2-Tetradecene, (E)-	196	C14H28	035953-54-9	91





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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
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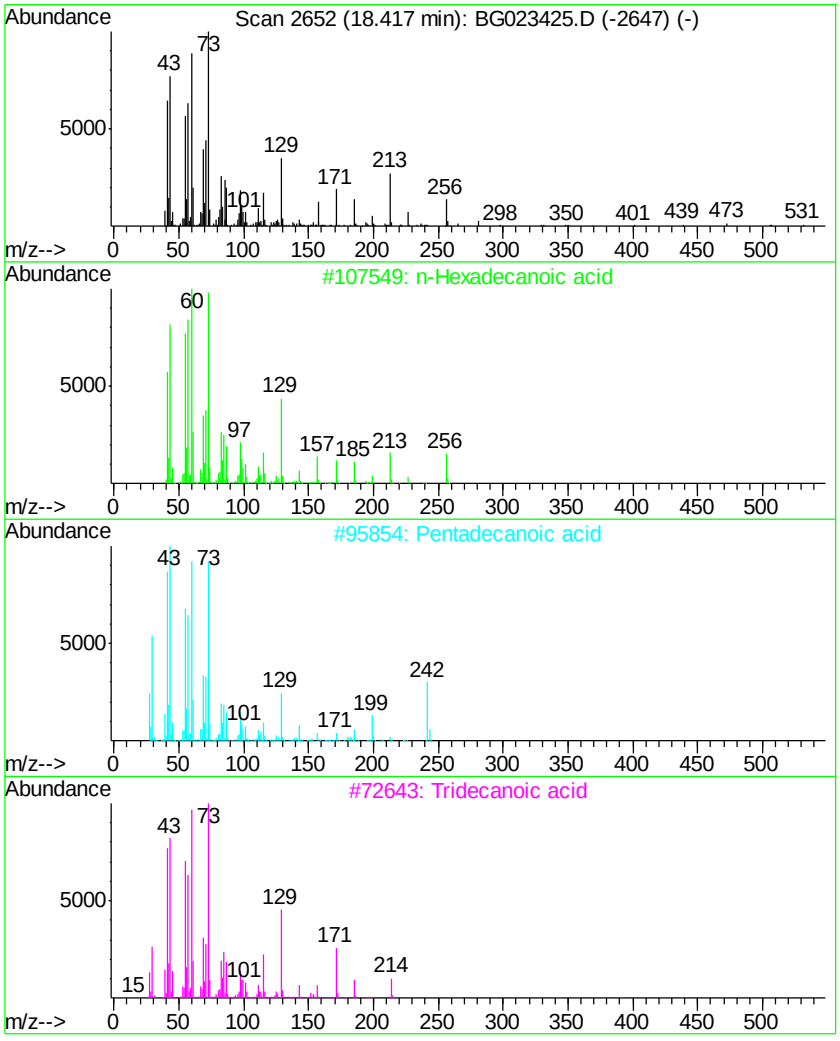
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

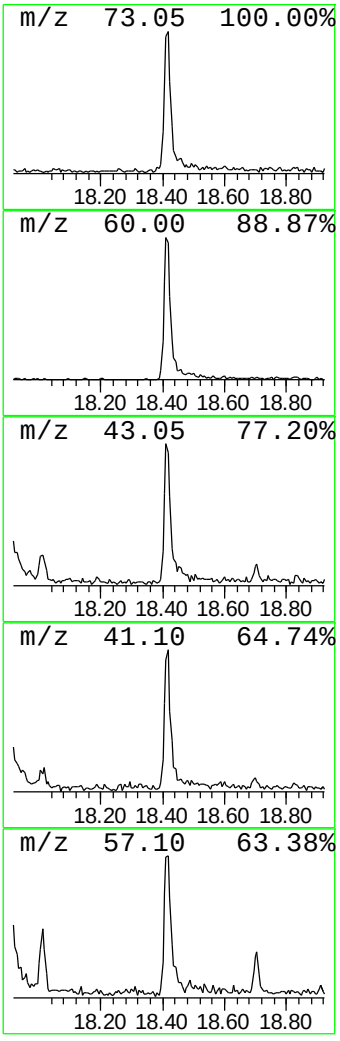
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	4.81 ng	565437	Phenanthrene-d10	17.54

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	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Octadecanoic acid	284	C18H36O2	000057-11-4	70
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

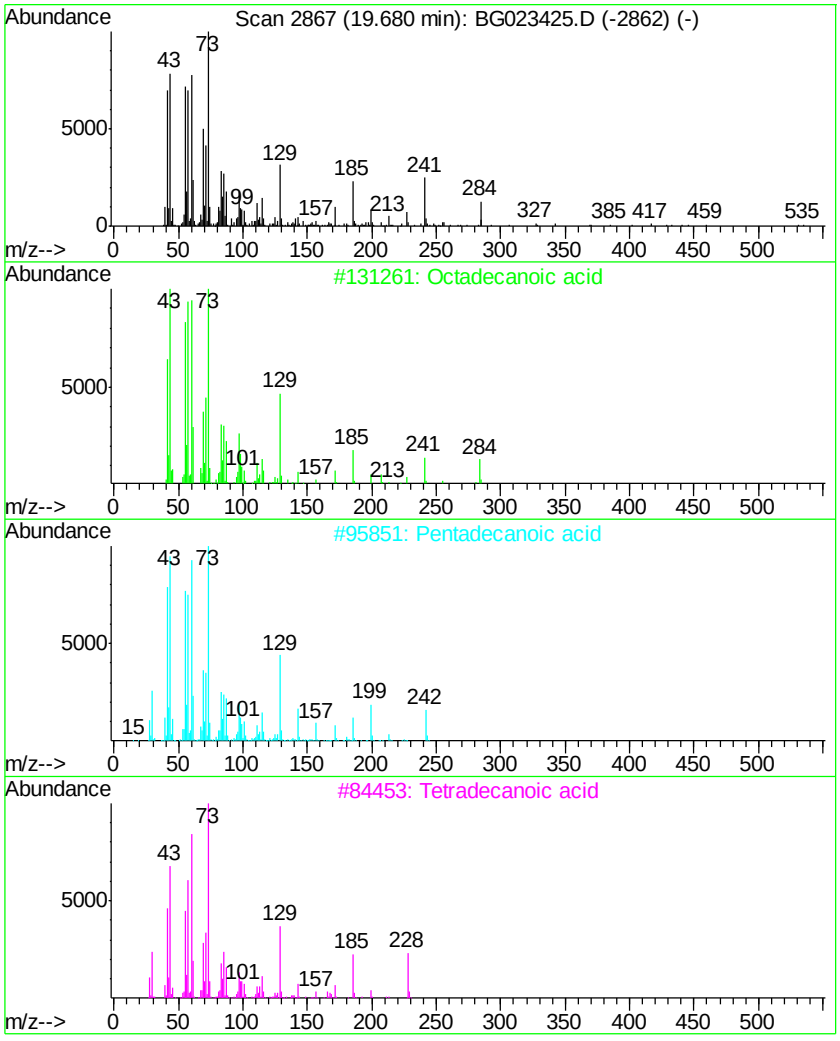
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

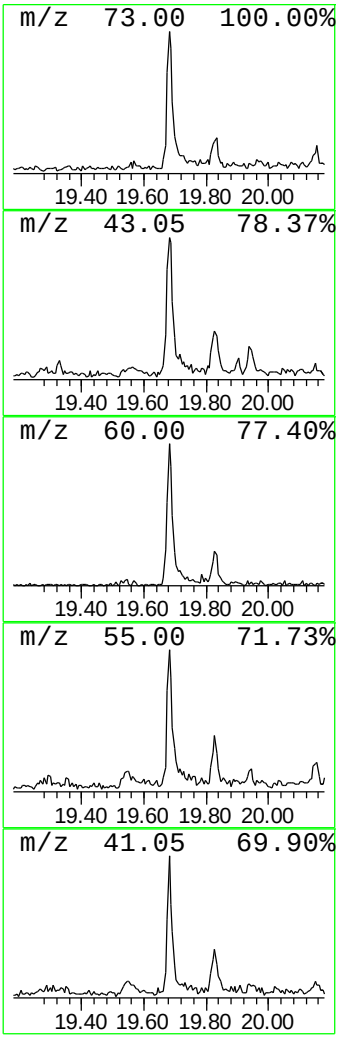
****

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.68	4.78 ng	562028	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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
Propane, 2,2-dime...	2.99	84.3	ng	2848230	1	8.12	675498	20.0
2-Pentanone, 4-hy...	5.18	21.9	ng	739356	1	8.12	675498	20.0
unknown7.64	7.64	94.8	ng	3200470	1	8.12	675498	20.0
Hexanoic acid, 2-...	9.41	3.0	ng	101426	1	8.12	675498	20.0
Cyclotetradecane	17.90	4.0	ng	476933	4	17.54	2352350	20.0
n-Hexadecanoic acid	18.42	4.8	ng	565437	4	17.54	2352350	20.0
Octadecanoic acid	19.68	4.8	ng	562028	4	17.54	2352350	20.0