LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015892.D
Acq On : 11 Jul 2018 17:08
Operator : SJ/JU
Sample : J3906-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-BOTTOM-1@3

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-BM070518.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	5.316	339	345	361	rVB	274750	432640	8.55%	1.185%
2	5.799	420	427	446	rBV	2254641	3405392	67.30%	9.330%
3	7.446	700	707	725	rBV	2243329	3736317	73.84%	10.237%
4	7.816	763	770	782	rBV	2430918	3880535	76.69%	10.632%
5	8.293	844	851	858	rBV	389276	644794	12.74%	1.767%
6	8.616	899	906	917	rBV	1677374	2729483	53.94%	7.478%
7	9.481	1045	1053	1066	rBV	1330992	2235501	44.18%	6.125%
8	11.122	1325	1332	1341	rBV	459305	800056	15.81%	2.192%
9	13.539	1736	1743	1753	rBV	2985928	4209262	83.18%	11.532%
10	14.357	1877	1882	1891	rBV	494534	681821	13.47%	1.868%
11	14.916	1970	1977	1984	rVB2	602817	939799	18.57%	2.575%
12	16.392	2222	2228	2242	rBV	2563349	3493235	69.03%	9.571%
13	17.639	2434	2440	2452	rBV	718992	1050734	20.76%	2.879%
14	18.480	2577	2583	2594	rBV	246144	372702	7.37%	1.021%
15	19.309	2719	2724	2730	rBV	41124	57582	1.14%	0.158%
16	19.727	2791	2795	2804	rBV	85230	121003	2.39%	0.332%
17	20.198	2870	2875	2885	rBV	4099876	5060182	100.00%	13.864%
18	21.415	3077	3082	3092	rVB2	169997	357811	7.07%	0.980%
19	21.503	3093	3097	3103	rVB	181296	218816	4.32%	0.600%
20	21.750	3134	3139	3144	rBV	760142	1019472	20.15%	2.793%
21	22.927	3335	3339	3346	rVB	82340	113112	2.24%	0.310%
22	24.144	3540	3546	3556	rVB2	492778	939304	18.56%	2.573%

Sum of corrected areas: 36499553

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
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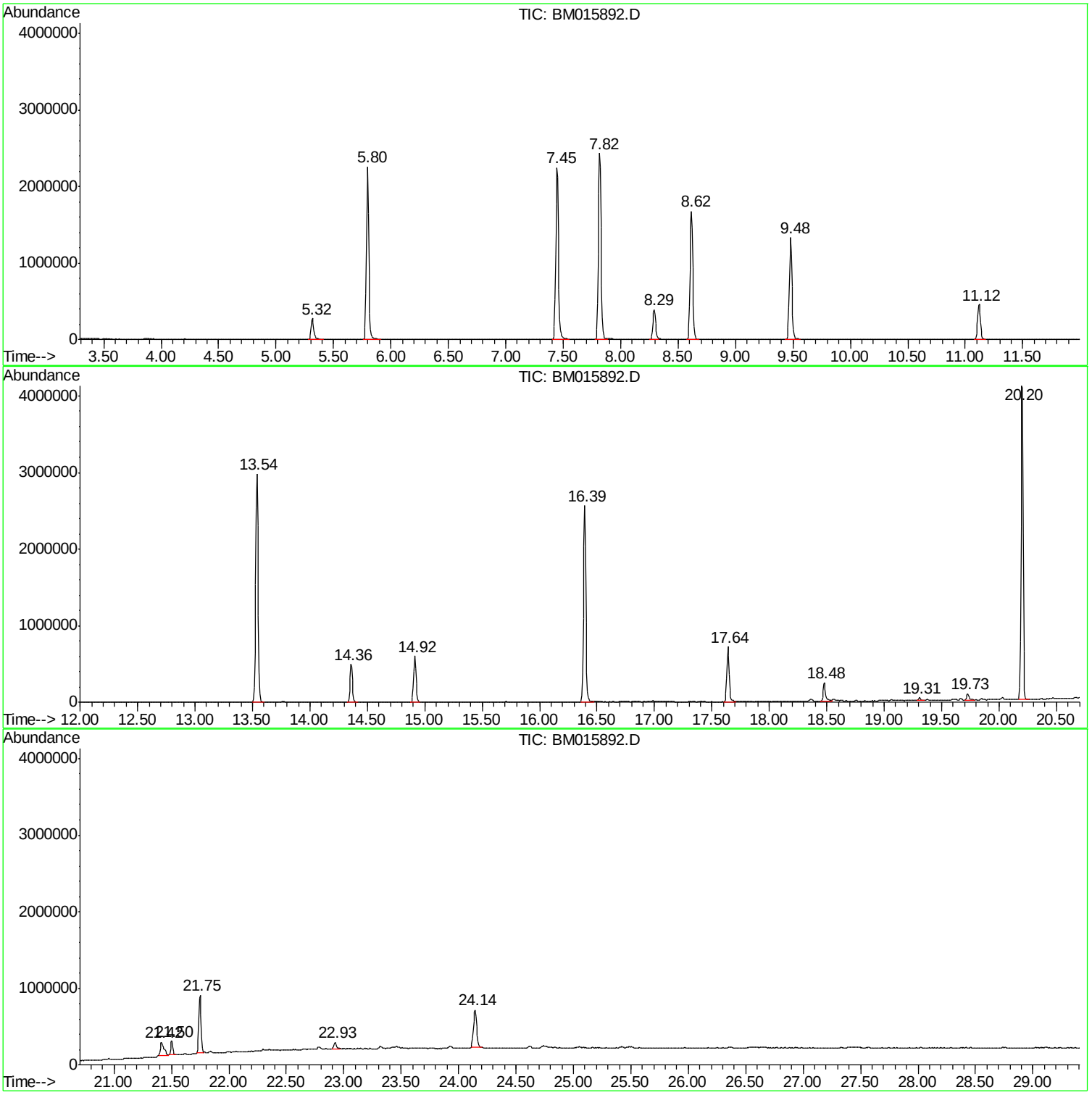
Sample : J3906-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB-7-8-6-ST-BOTTOM-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015892.D
Acq On : 11 Jul 2018 17:08
Operator : SJ/JU
Sample : J3906-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-BOTTOM-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

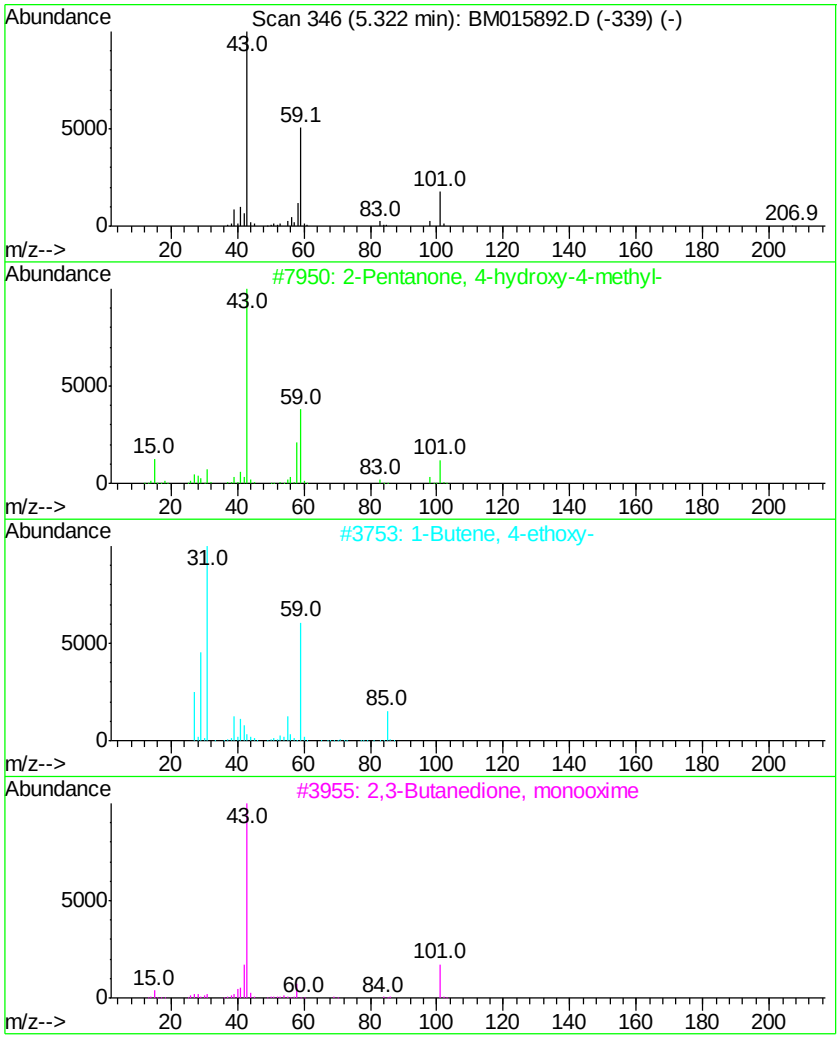
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

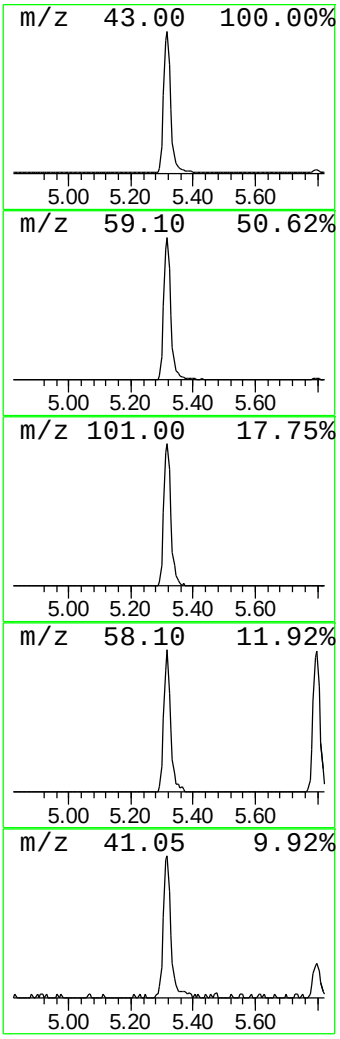
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	13.42 ng	432640	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Propylamine	59	C3H9N	000107-10-8	9
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

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Operator : SJ/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-BOTTOM-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

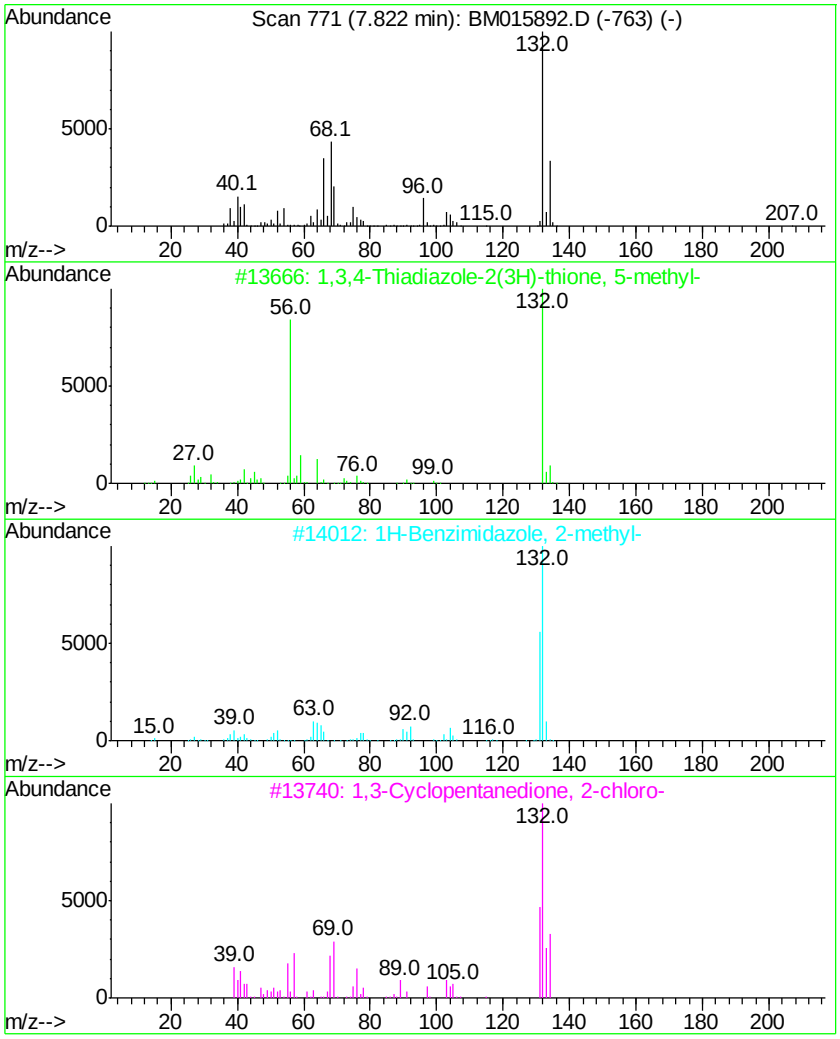
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

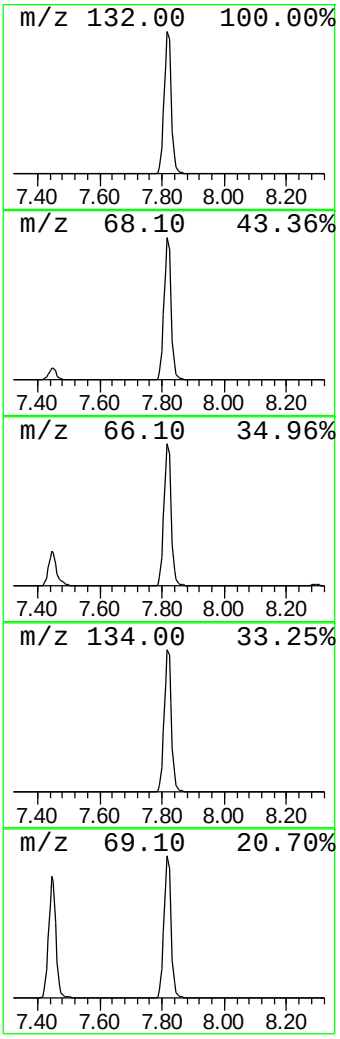
****

Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	120.37 ng	3880540	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





Library Search Compound Report

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Data File : BM015892.D
Acq On : 11 Jul 2018 17:08
Operator : SJ/JU
Sample : J3906-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-BOTTOM-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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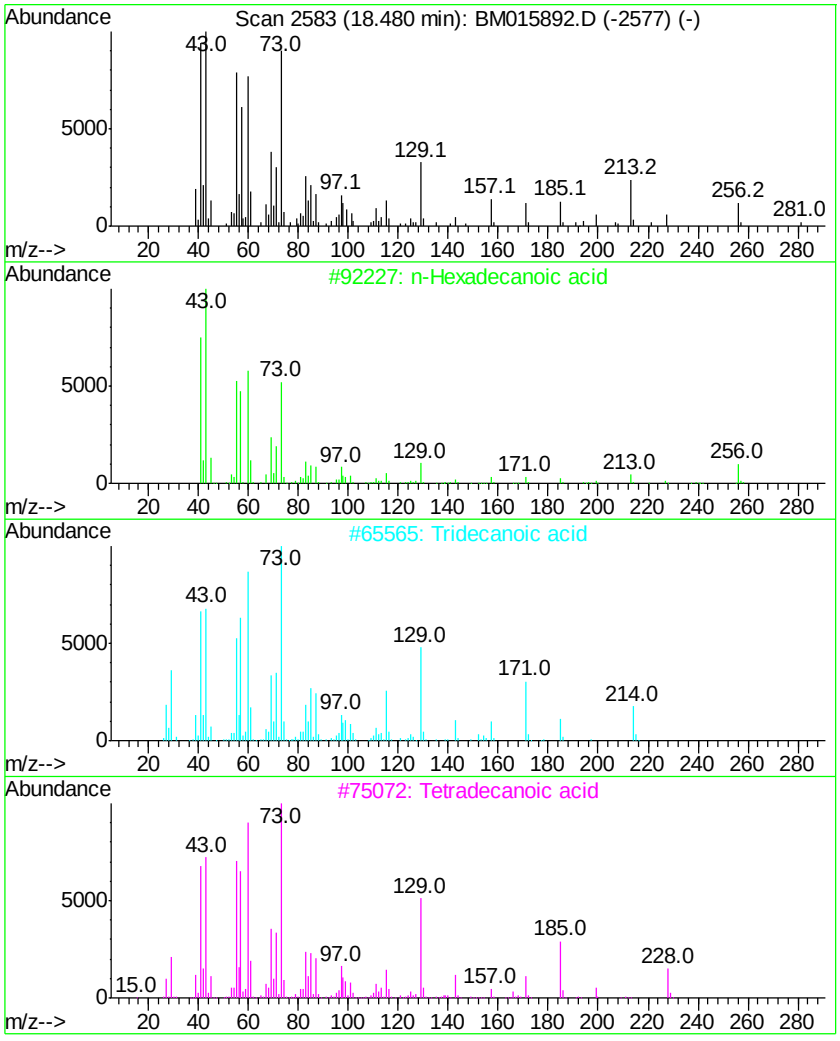
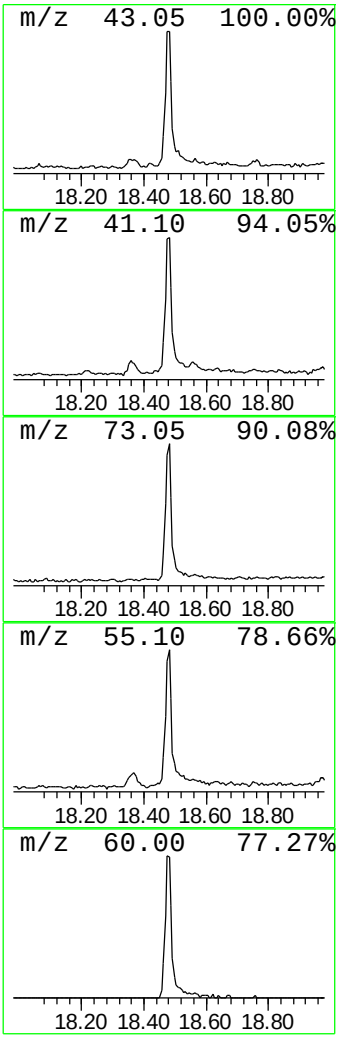
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.48	7.09 ng	372702	Phenanthrene-d10	17.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Undecanoic acid	186	C11H22O2	000112-37-8	50
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	46





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Data File : BM015892.D
Acq On : 11 Jul 2018 17:08
Operator : SJ/JU
Sample : J3906-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-BOTTOM-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

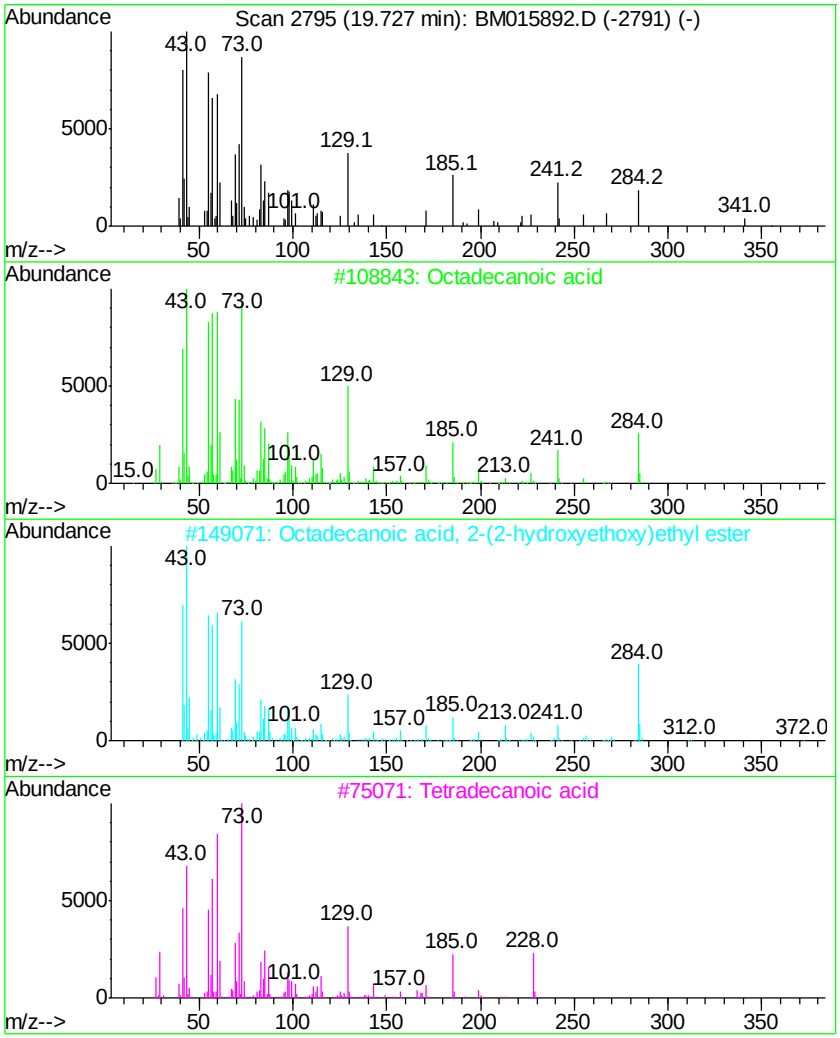
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

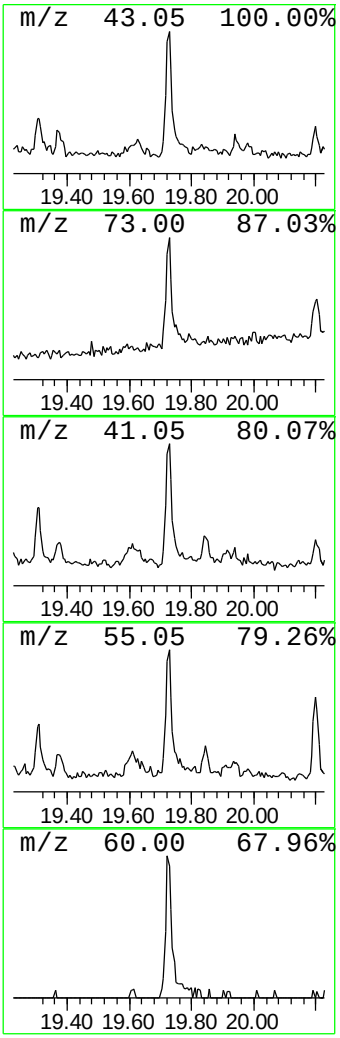
****

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	2.37 ng	121003	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	53
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4	Octadecanoic acid, 2-hydroxy-1,3...	625	C39H76O5	000504-40-5	47
5	Tridecanoic acid	214	C13H26O2	000638-53-9	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
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Acq On : 11 Jul 2018 17:08
Operator : SJ/JU
Sample : J3906-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-BOTTOM-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

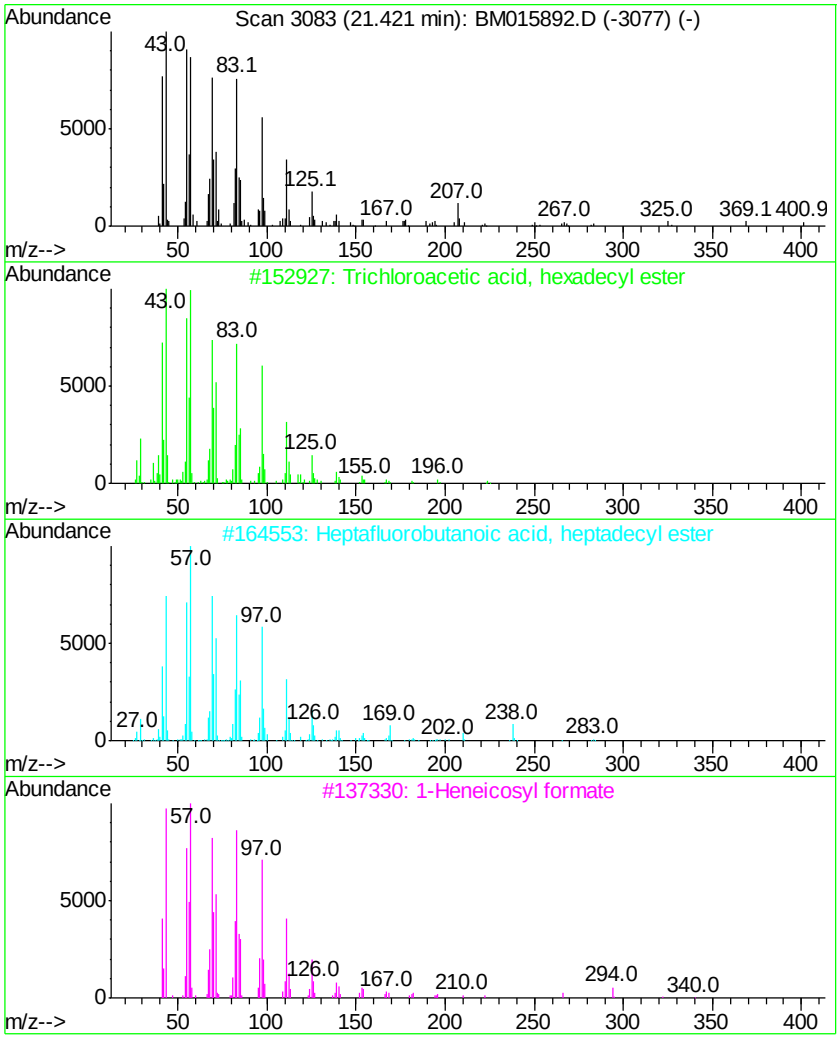
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

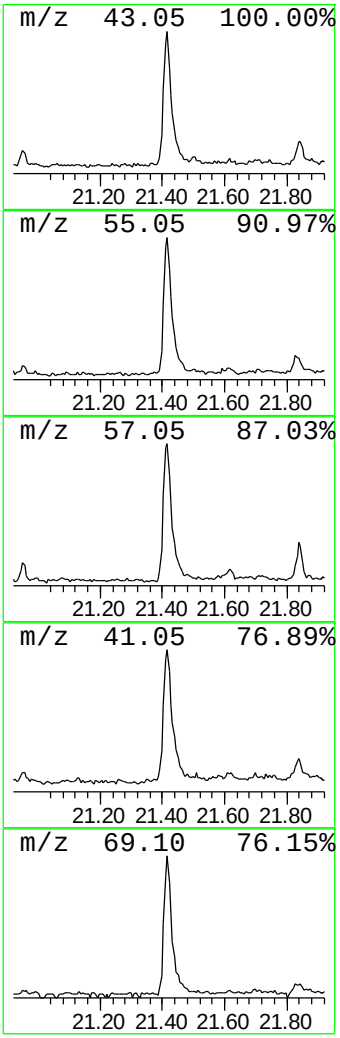
****

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	7.02 ng	357811	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91





Library Search Compound Report

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Instrument : BNA_M
ClientSampleId : CB-7-8-6-ST-BOTTOM-1@3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

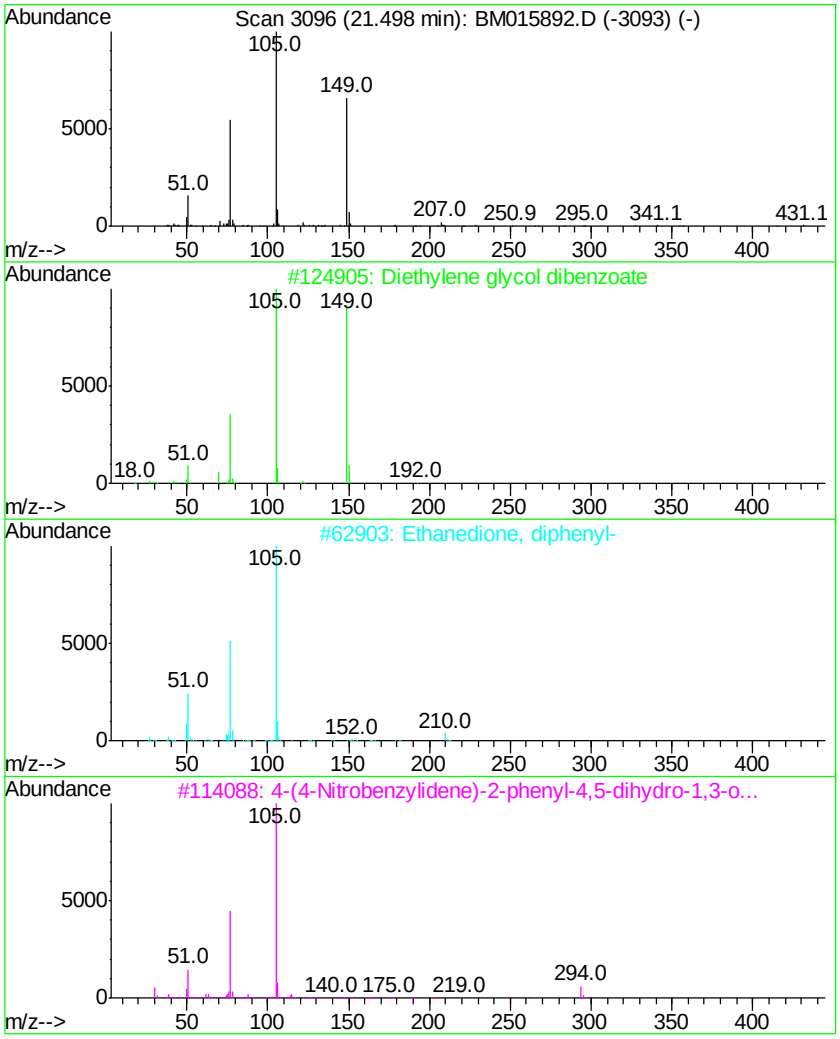
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

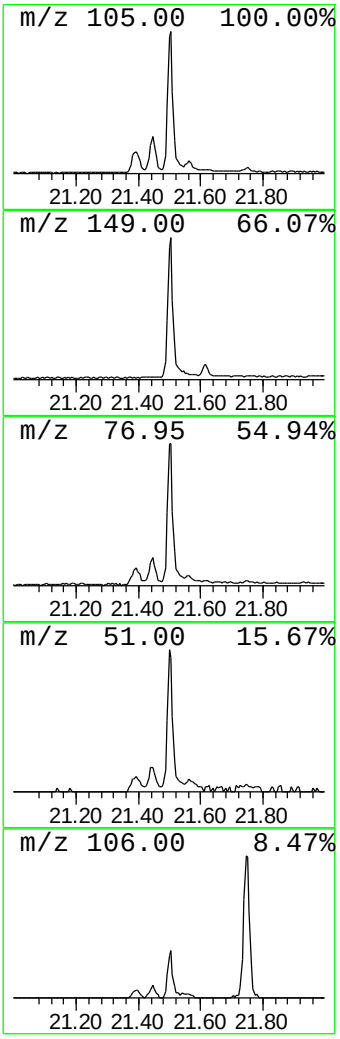
****

Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	4.29 ng	218816	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	59
2	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	47
3	4-(4-Nitrobenzylidene)-2-phenyl-...	294	C16H10N2O4	007152-75-2	47
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47





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Instrument : BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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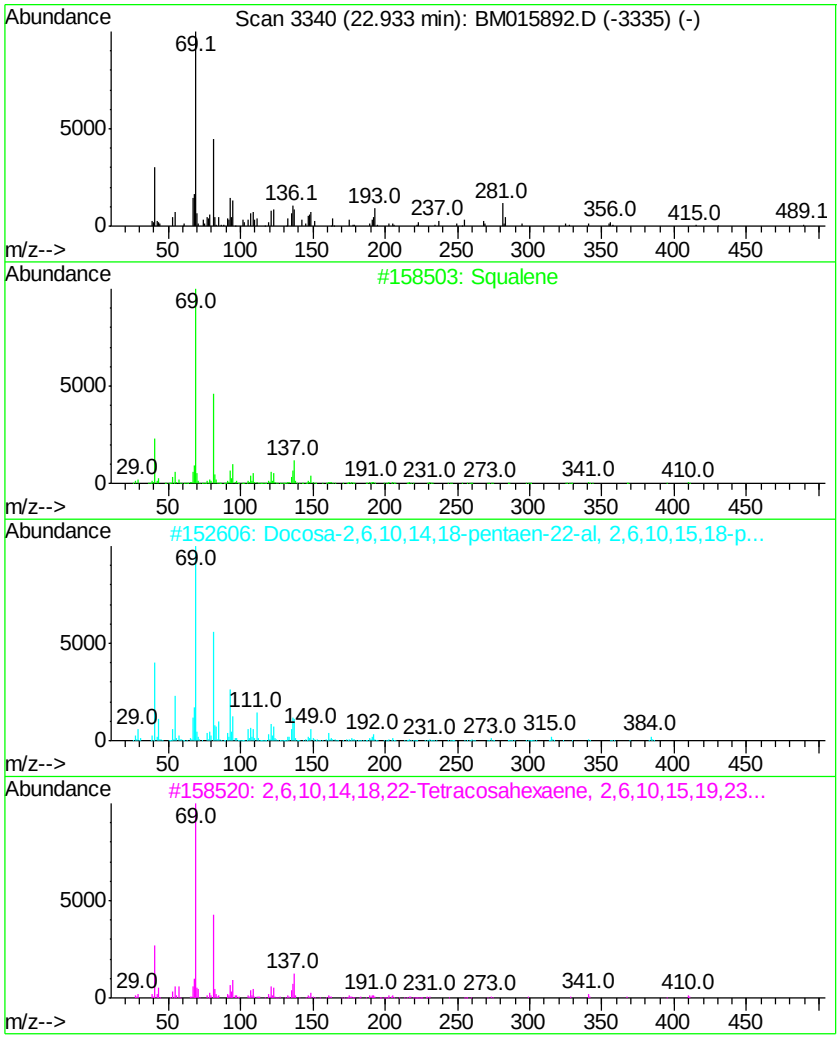
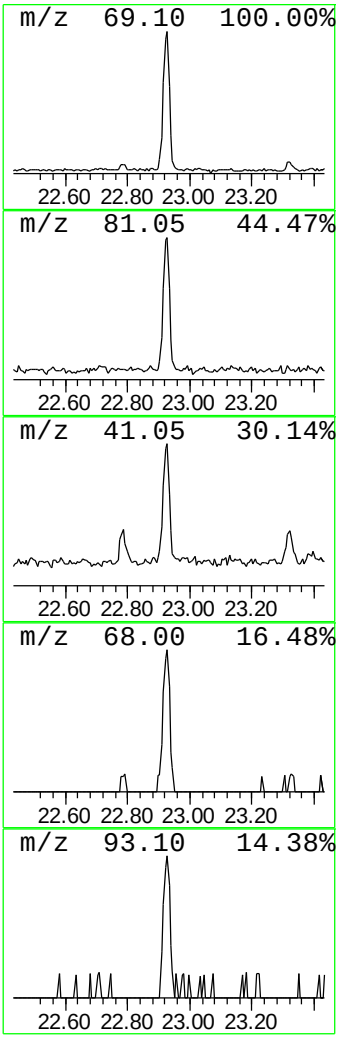
Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.93	2.22 ng	113112	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	83
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
3	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	80
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.32	13.4	ng	432640	1	8.29	644794	20.0
unknown7.82	7.82	120.4	ng	3880540	1	8.29	644794	20.0
n-Hexadecanoic acid	18.48	7.1	ng	372702	4	17.64	1050730	20.0
Octadecanoic acid	19.73	2.4	ng	121003	5	21.75	1019470	20.0
Trichloroacetic a...	21.42	7.0	ng	357811	5	21.75	1019470	20.0
Diethylene glycol...	21.50	4.3	ng	218816	5	21.75	1019470	20.0
Squalene	22.93	2.2	ng	113112	5	21.75	1019470	20.0