LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084638.D
Acq On : 29 Jan 2016 16:13
Operator : SJ/IZ
Sample : H1257-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B015(10-13)

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-BF012916.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	4.190	181	184	193	rBV	315660	481598	8.75%	1.023%
2	4.899	241	246	248	rBV	3332675	5503694	100.00%	11.685%
3	5.322	280	283	286	rBV	3952606	3894229	70.76%	8.268%
4	5.722	316	318	321	rBV	358785	363128	6.60%	0.771%
5	6.373	372	375	377	rBV	4374696	4485436	81.50%	9.523%
6	6.487	383	385	388	rBV	3068694	4239788	77.04%	9.002%
7	6.727	403	406	408	rBV	882189	1009393	18.34%	2.143%
8	6.876	417	419	422	rBV	3120172	3039929	55.23%	6.454%
9	7.287	453	455	458	rBV	2452146	2463469	44.76%	5.230%
10	8.008	516	518	520	rBV	1648062	1367761	24.85%	2.904%
11	9.093	610	613	615	rBV	4401726	4902357	89.07%	10.408%
12	9.482	645	647	650	rBV	492572	466524	8.48%	0.990%
13	9.699	664	666	669	rBV	43535	58771	1.07%	0.125%
14	9.756	669	671	674	rBV	1487873	1454558	26.43%	3.088%
15	10.202	709	710	712	rVB	165701	123507	2.24%	0.262%
16	10.419	726	729	732	rBV	50080	83165	1.51%	0.177%
17	10.545	738	740	743	rBV	2928875	3003641	54.57%	6.377%
18	10.671	750	751	756	rBV	148254	196298	3.57%	0.417%
19	11.116	789	790	792	rBV	54177	70521	1.28%	0.150%
20	11.242	799	801	802	rBV	1517589	1503304	27.31%	3.192%
21	11.779	846	848	850	rBV2	33306	55623	1.01%	0.118%
22	12.442	904	906	908	rBV	67930	69550	1.26%	0.148%
23	12.671	923	926	929	rBV	80860	86369	1.57%	0.183%
24	12.831	937	940	942	rBV	4905730	4857765	88.26%	10.314%
25	13.757	1018	1021	1028	rBV	175222	506410	9.20%	1.075%
26	13.871	1028	1031	1033	rBV	1504968	1444970	26.25%	3.068%
27	14.351	1067	1073	1076	rBV5	20067	73504	1.34%	0.156%
28	14.717	1103	1105	1108	rBV	174065	175237	3.18%	0.372%
29	15.254	1149	1152	1155	rBV	912612	1022453	18.58%	2.171%
30	15.814	1195	1201	1206	rBV6	24447	96977	1.76%	0.206%

Sum of corrected areas: 47099929

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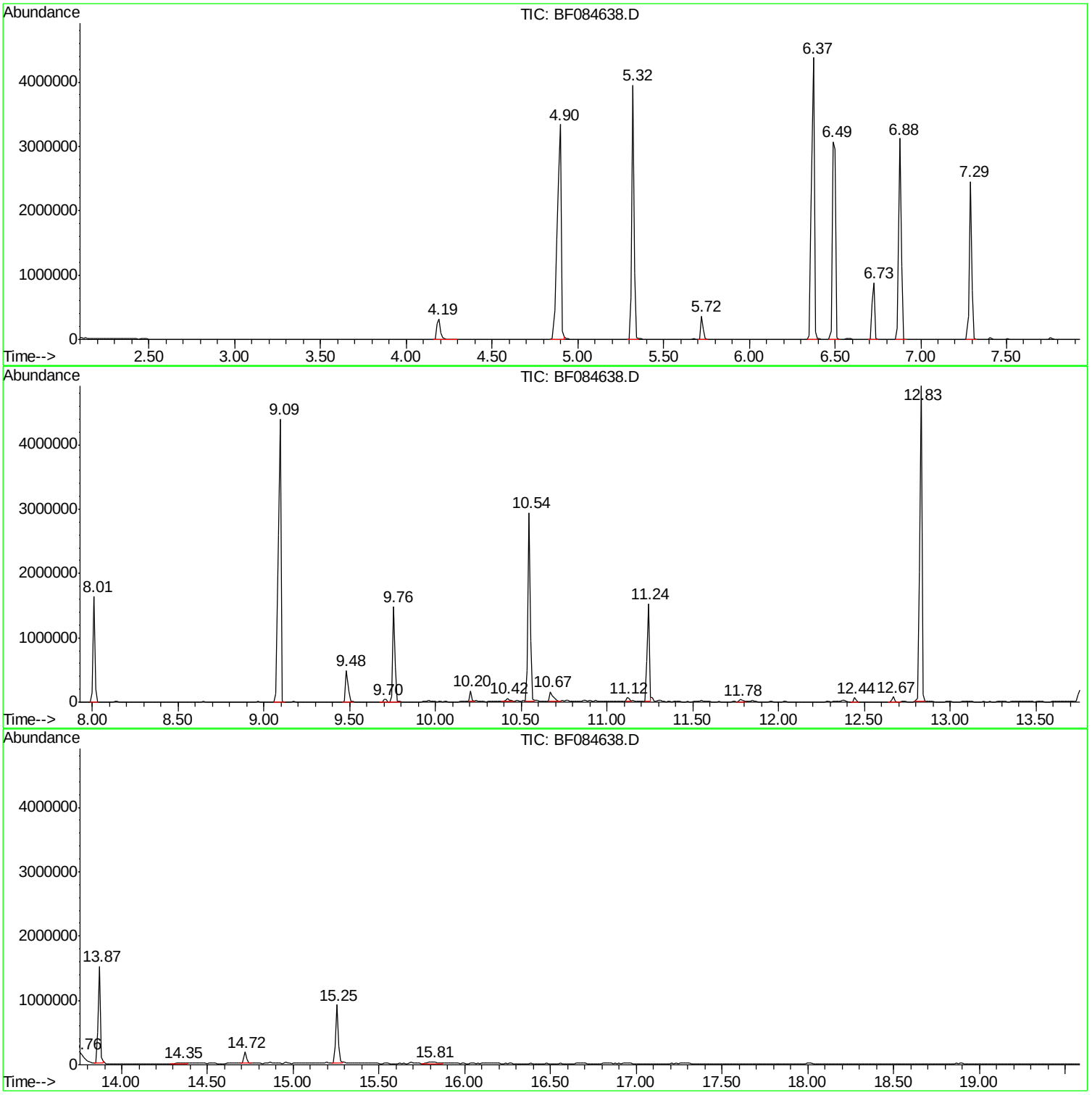
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-B015(10-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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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Data File : BF084638.D
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

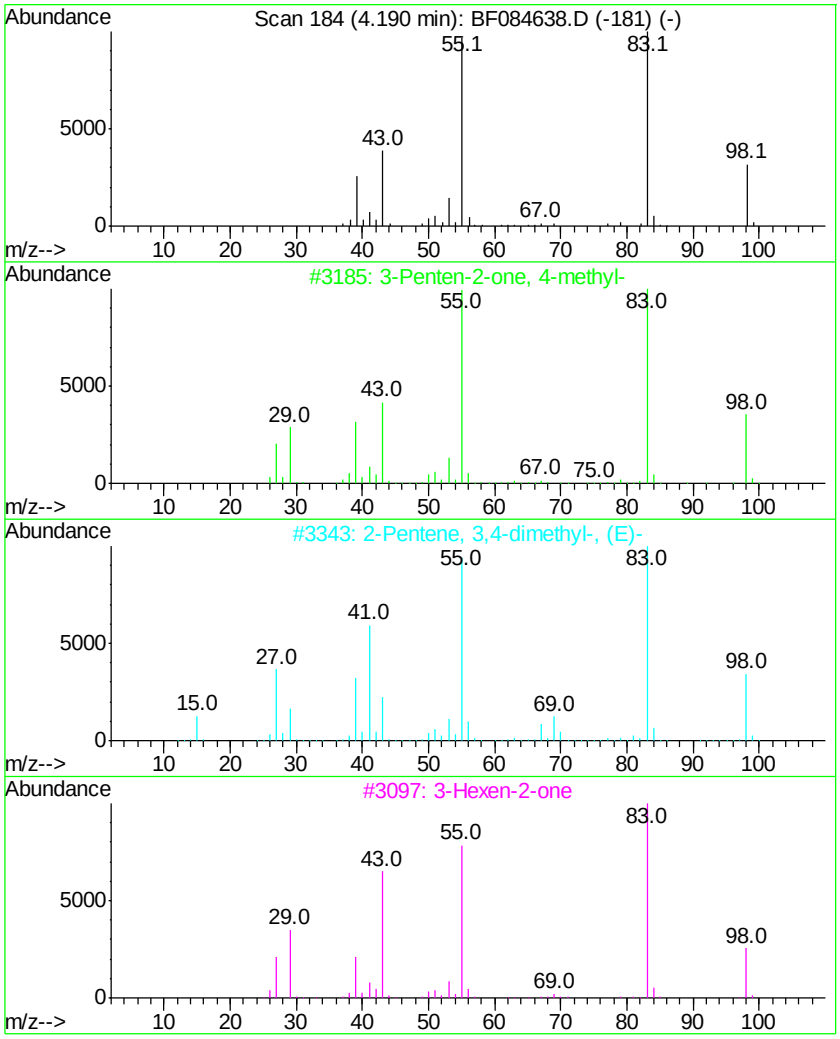
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

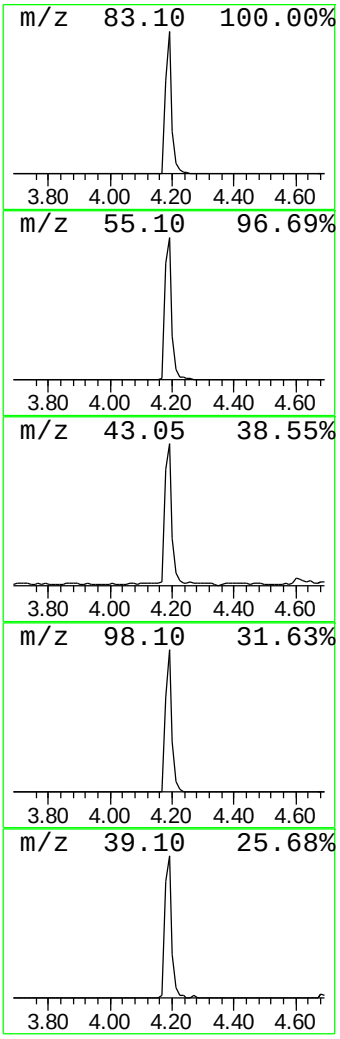
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	9.54 ng	481598	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Operator : SJ/IZ
Sample : H1257-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B015(10-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

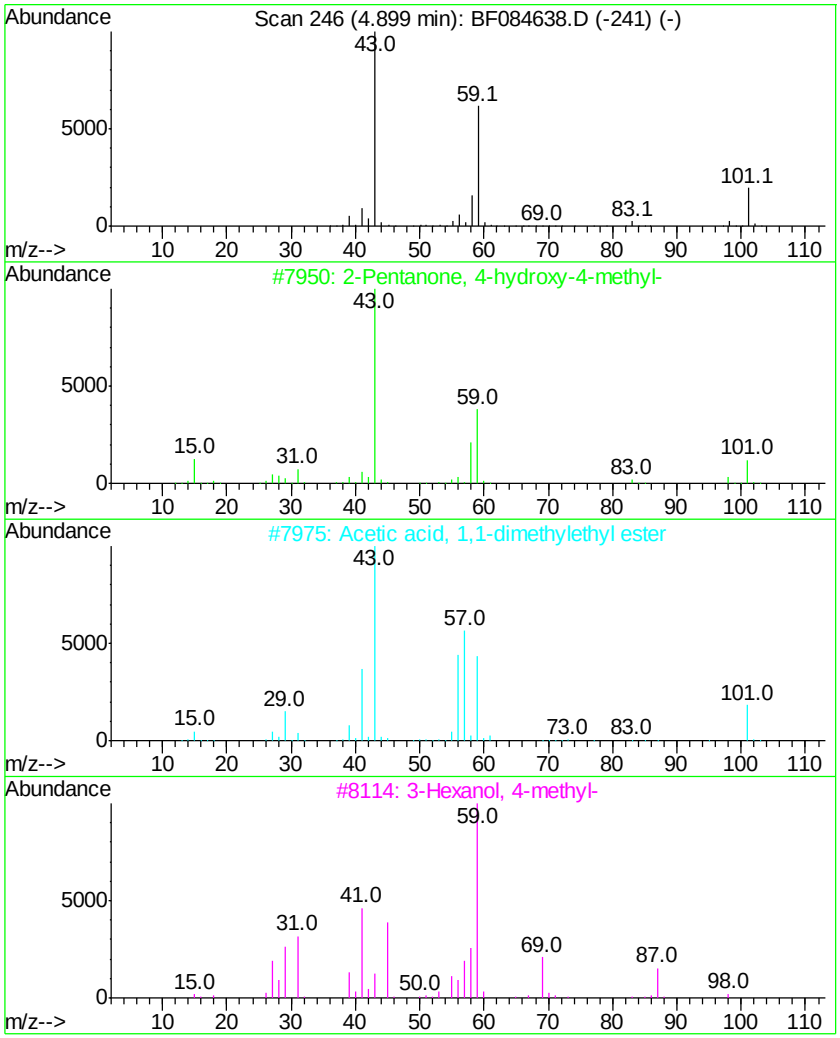
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

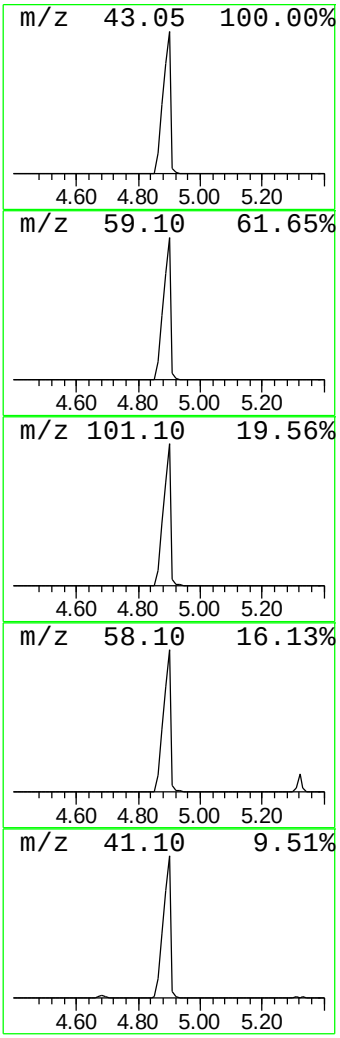
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	109.05 ng	5503690	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
Data File : BF084638.D
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Operator : SJ/IZ
Sample : H1257-05
Misc :
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Instrument : BNA_F
ClientSampleId : SUP-B015(10-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
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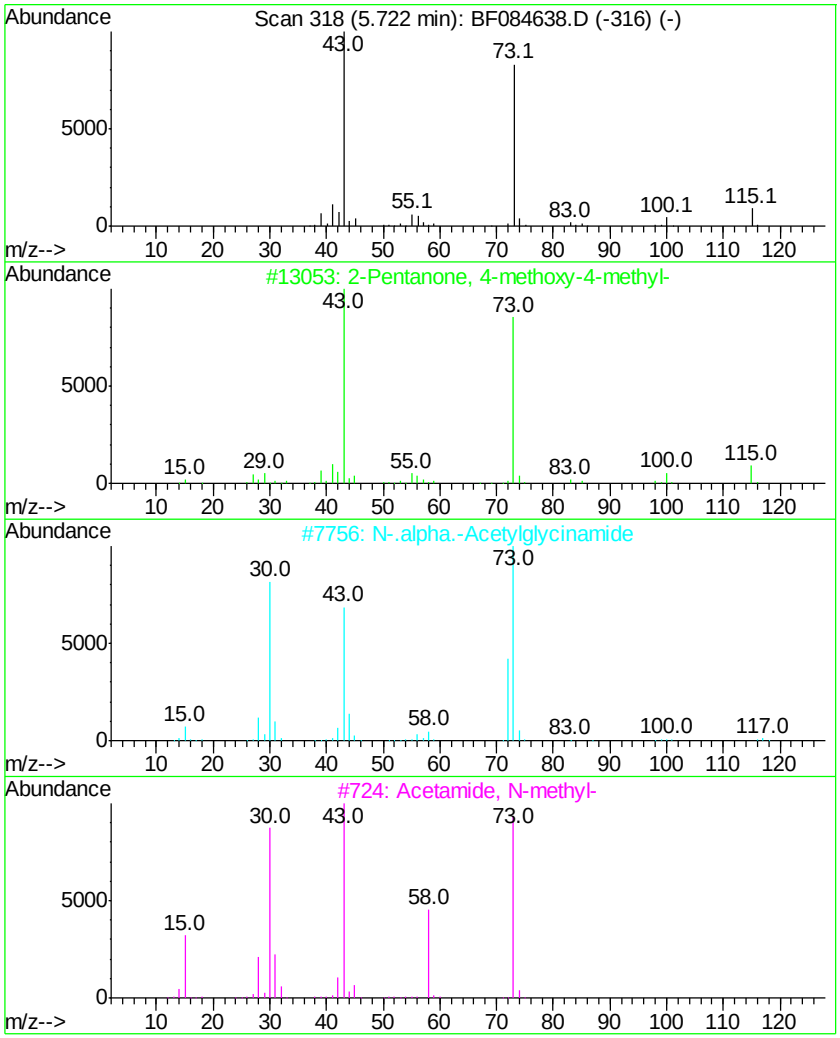
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

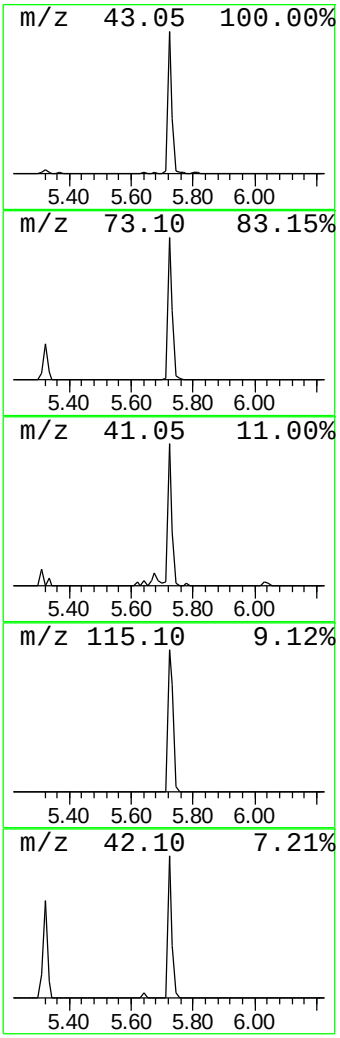
****

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	7.19 ng	363128	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10





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Data File : BF084638.D
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Operator : SJ/IZ
Sample : H1257-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B015(10-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
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TIC Library : C:\DATABASE\NIST02.L
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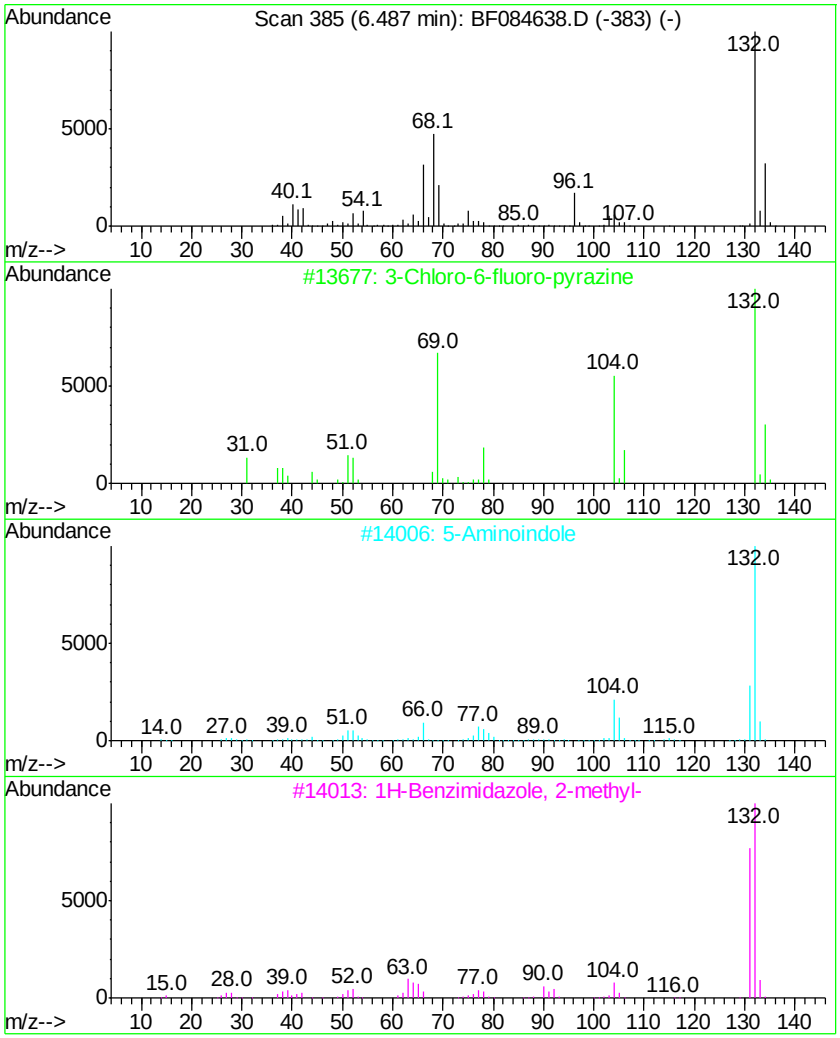
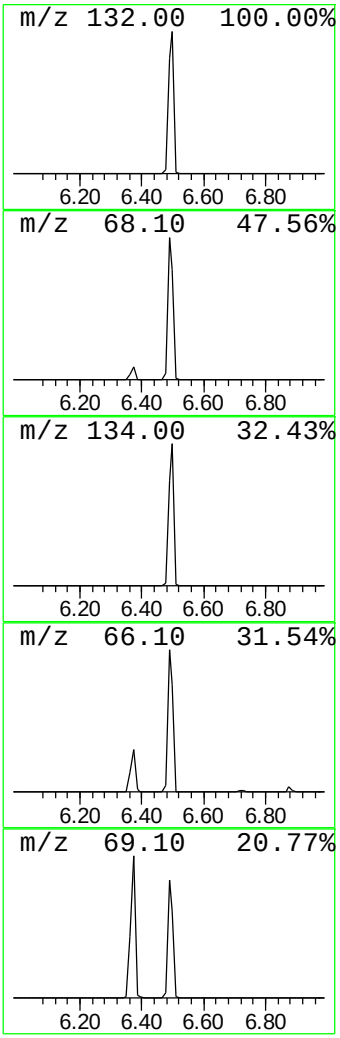
Peak Number 4 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	84.01 ng	4239790	1,4-Dichlorobenzene-d4	6.73

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	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012916\
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Sample : H1257-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B015(10-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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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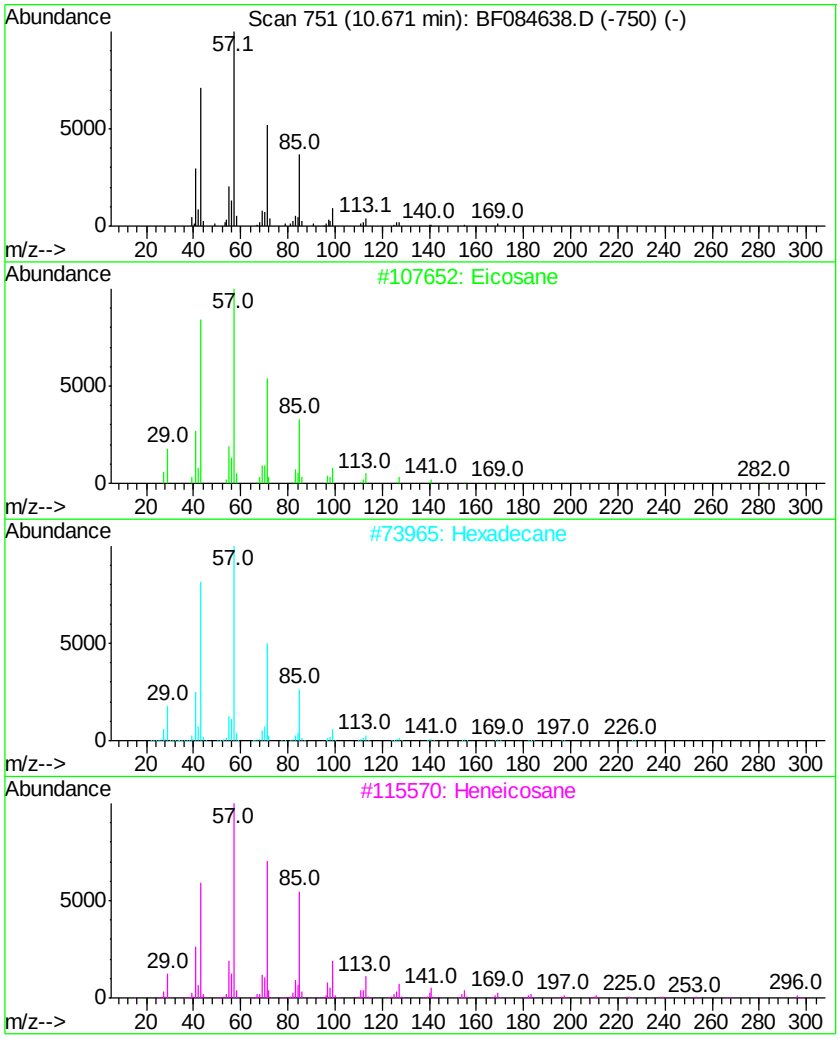
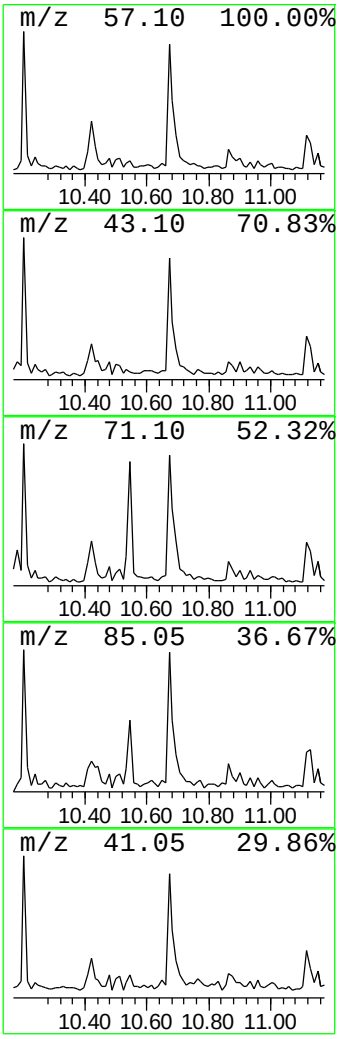
Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.61 ng	196298	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	83
4	Pentadecane	212	C15H32	000629-62-9	83
5	Tetradecane	198	C14H30	000629-59-4	64





Library Search Compound Report

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Sample : H1257-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B015(10-13)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.M
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TIC Library : C:\DATABASE\NIST02.L
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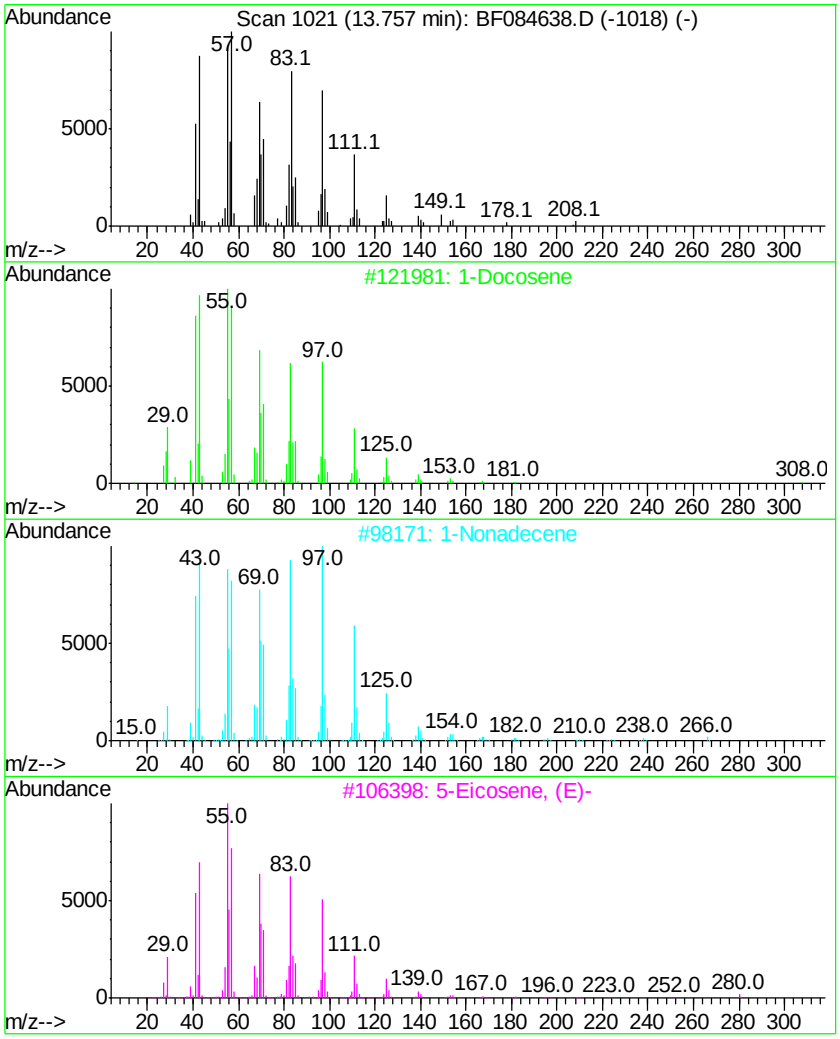
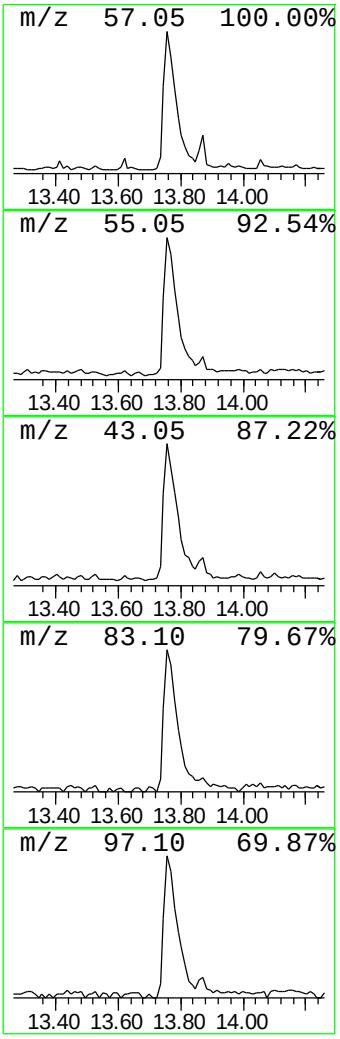
Peak Number 7 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	7.01 ng	506410	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	87
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	86
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	81





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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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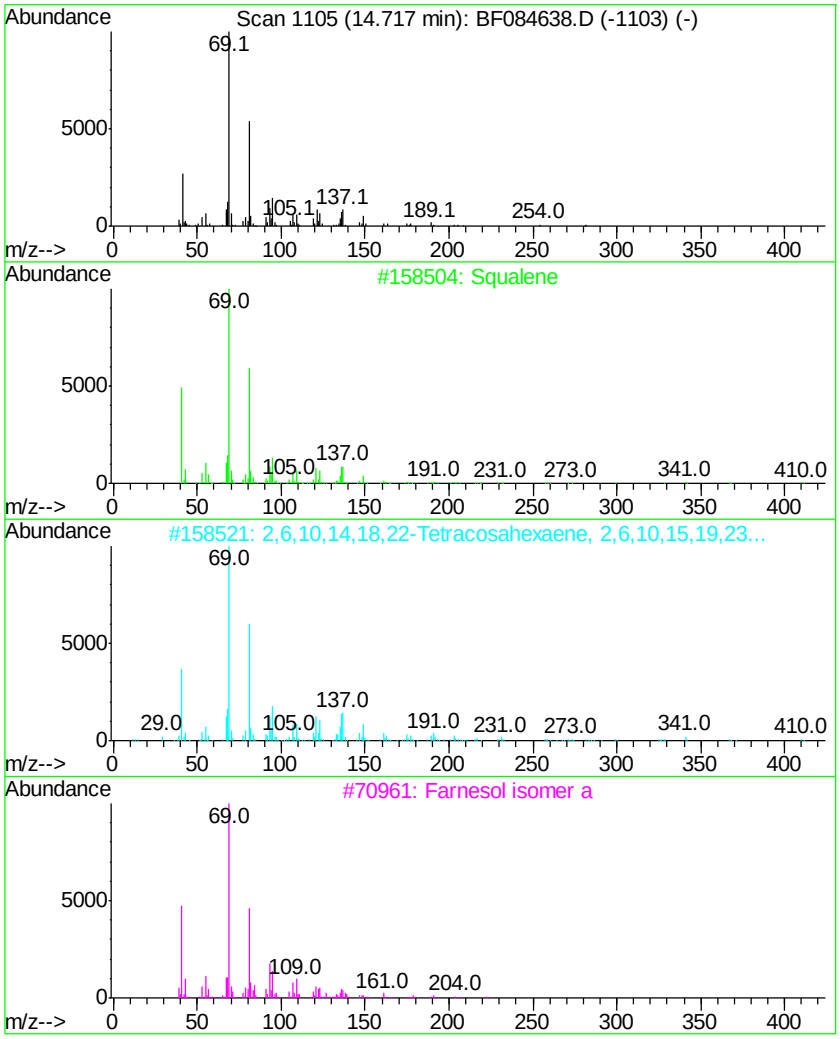
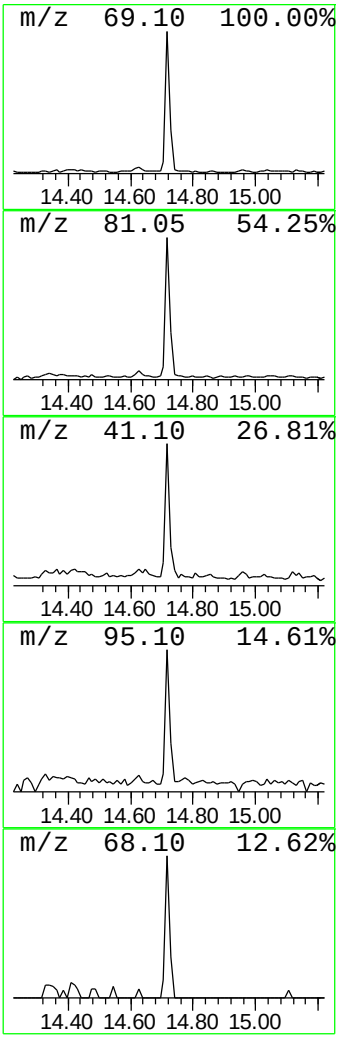
Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.43 ng	175237	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	Farnesol isomer a	222	C15H26O	1000108-92-4	72
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53
5	Trideca-1,7,11-triene-1,1-dicarb...	270	C18H26N2	1000161-46-0	53





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.19	9.5	ng	481598	1	6.73	1009390	20.0
2-Pentanone, 4-hy...	4.90	109.1	ng	5503690	1	6.73	1009390	20.0
2-Pentanone, 4-me...	5.72	7.2	ng	363128	1	6.73	1009390	20.0
unknown6.49	6.49	84.0	ng	4239790	1	6.73	1009390	20.0
Eicosane	10.67	2.6	ng	196298	4	11.24	1503300	20.0
1-Docosene	13.76	7.0	ng	506410	5	13.87	1444970	20.0
Squalene	14.72	3.4	ng	175237	6	15.25	1022450	20.0