LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

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-BF103015.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	4.373	198	200	207	rBV2	134291	223904	4.71%	0.488%
2	4.853	240	242	249	rBV	149735	173136	3.64%	0.378%
3	5.059	256	260	262	rBV	1387331	2125851	44.72%	4.635%
4	5.470	294	296	299	rBV	2825999	3893717	81.91%	8.490%
5	6.510	383	387	389	rBV	3296068	4535493	95.41%	9.890%
6	6.647	396	399	401	rBV	3889536	4396153	92.48%	9.586%
7	6.876	417	419	421	rVB	1577841	1251687	26.33%	2.729%
8	7.036	430	433	435	rBV	3988055	3443461	72.44%	7.508%
9	7.436	465	468	470	rBV	2962245	2688171	56.55%	5.862%
10	8.167	529	532	534	rBV	1461720	1556625	32.75%	3.394%
11	9.242	624	626	629	rVB	5272414	4753489	100.00%	10.365%
12	9.630	658	660	663	rBV	590353	639318	13.45%	1.394%
13	9.859	679	680	683	rBV	66660	90280	1.90%	0.197%
14	9.916	683	685	687	rBV	1867498	1768719	37.21%	3.857%
15	10.362	723	724	726	rVB	220805	170968	3.60%	0.373%
16	10.579	740	743	747	rBV	52465	103837	2.18%	0.226%
17	10.705	752	754	756	rVV	3706310	3335803	70.18%	7.274%
18	10.842	764	766	772	rBV	132997	254733	5.36%	0.555%
19	11.288	800	805	806	rBV	105115	115489	2.43%	0.252%
20	11.402	813	815	817	rBV	2210512	1901643	40.01%	4.146%
21	11.471	818	821	823	rBV	39990	58399	1.23%	0.127%
22	11.939	860	862	864	rBV2	160141	167540	3.52%	0.365%
23	12.191	882	884	887	rBV	69679	68488	1.44%	0.149%
24	12.614	919	921	923	rBV	87498	91977	1.93%	0.201%
25	12.728	928	931	933	rBV2	36397	56018	1.18%	0.122%
26	12.842	938	941	943	rVB	66199	82527	1.74%	0.180%
27	12.991	952	954	957	rBV	4784390	4752354	99.98%	10.362%
28	13.905	1031	1034	1041	rBV	135183	258639	5.44%	0.564%
29	14.042	1043	1046	1048	rBV	1532344	1535331	32.30%	3.348%
30	14.922	1120	1123	1125	rBV	149301	177528	3.73%	0.387%
31	15.071	1134	1136	1143	rBV	25580	62931	1.32%	0.137%
32	15.494	1169	1173	1175	rBV	733743	1127275	23.71%	2.458%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

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-BF103015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

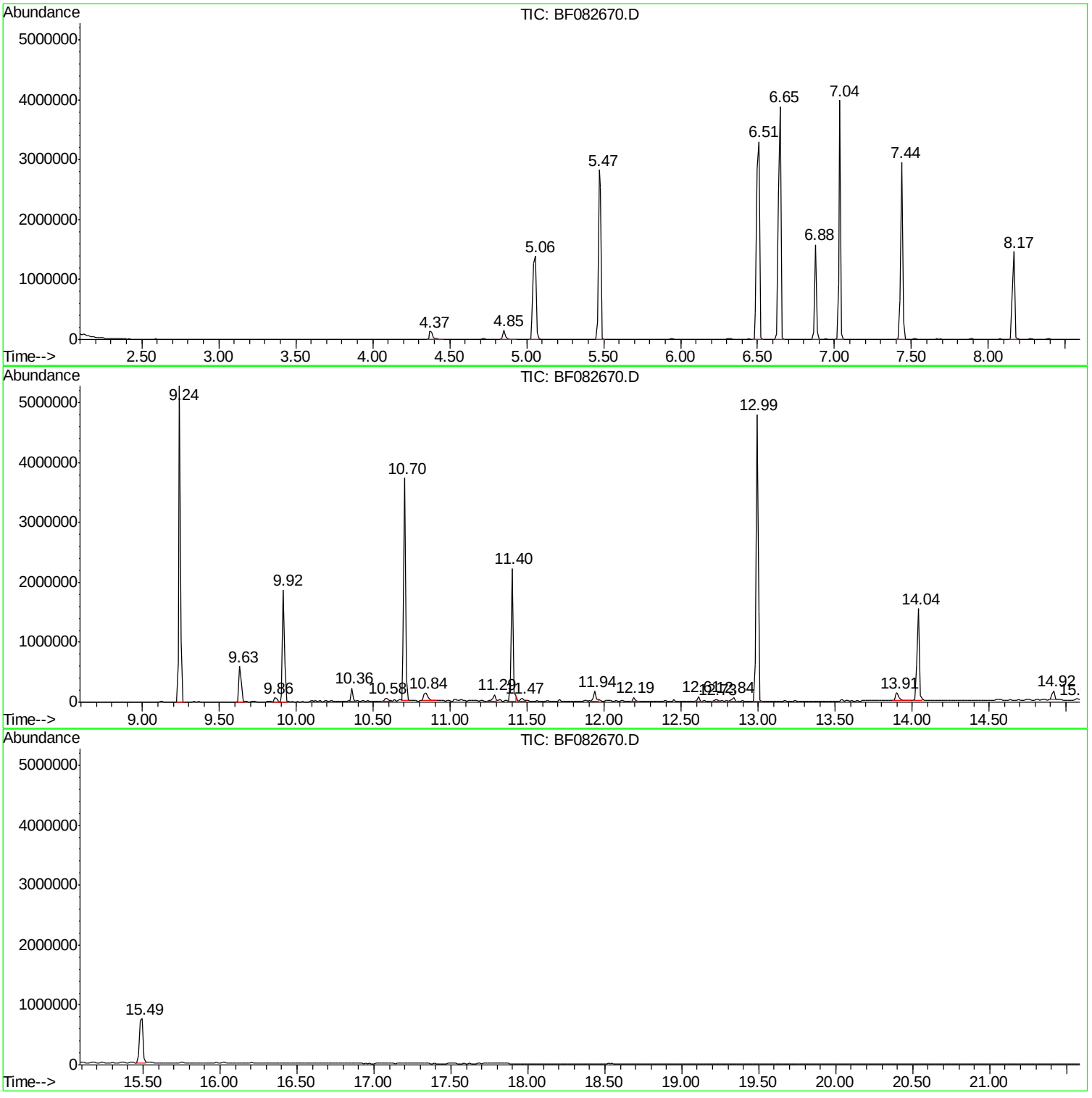
Sum of corrected areas: 45861484

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.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:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

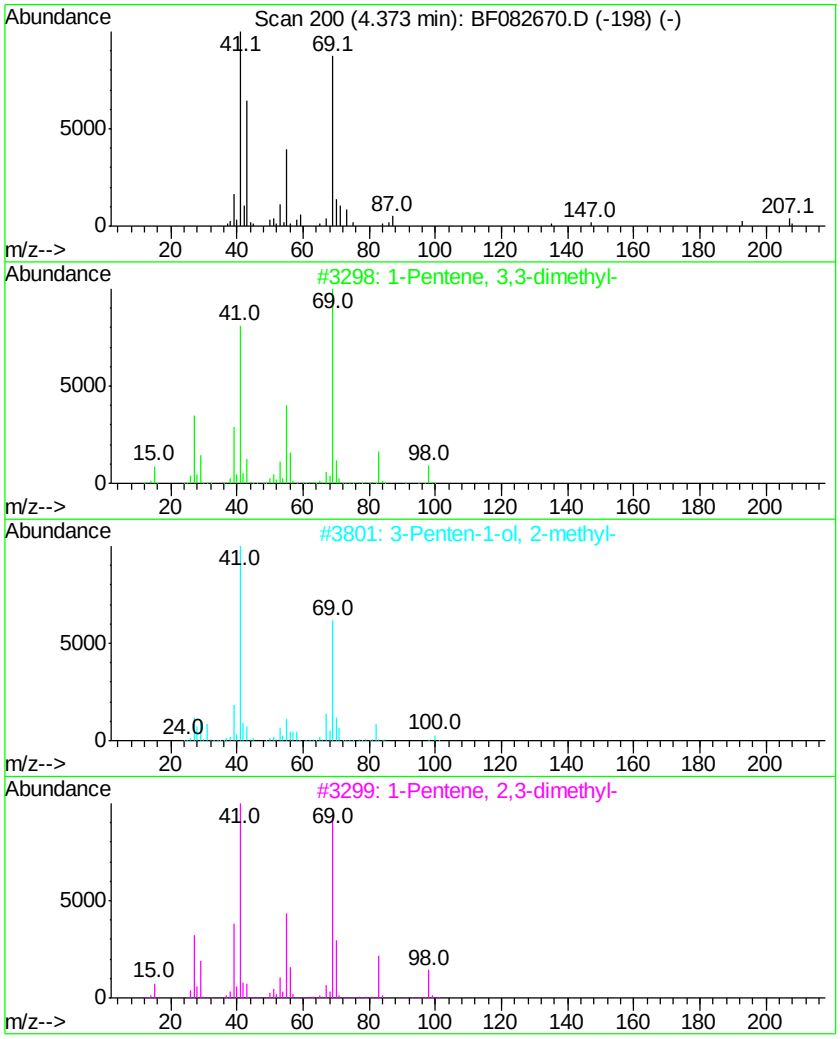
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

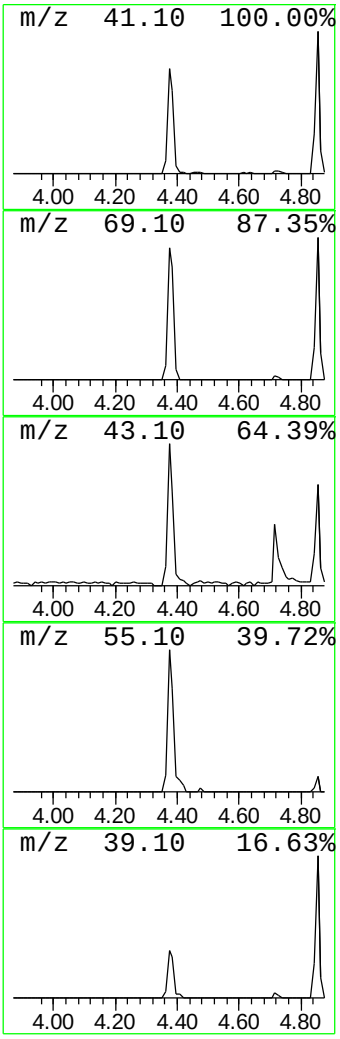
****

Peak Number 1 unknown4.37 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	3.58 ng	223904	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	45
2	3-Penten-1-ol, 2-methyl-	100	C6H12O	062238-37-3	45
3	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	42
4	2-Butene, 1-bromo-3-methyl-	148	C5H9Br	000870-63-3	40
5	2-Pentene, 4,4'-oxybis-	154	C10H18O	052867-34-2	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

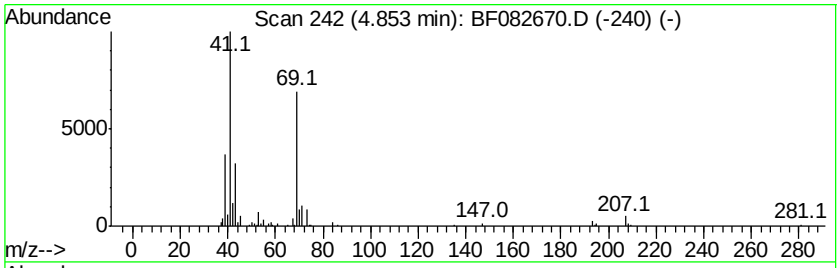
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

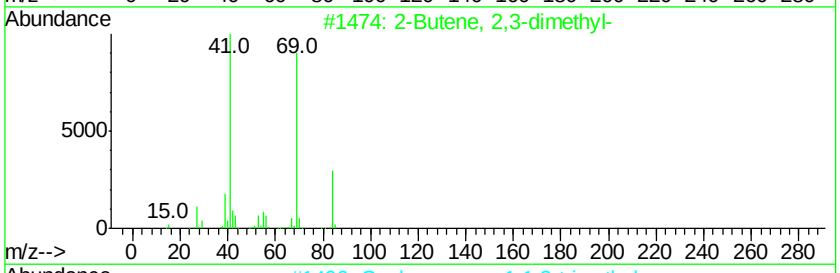
****

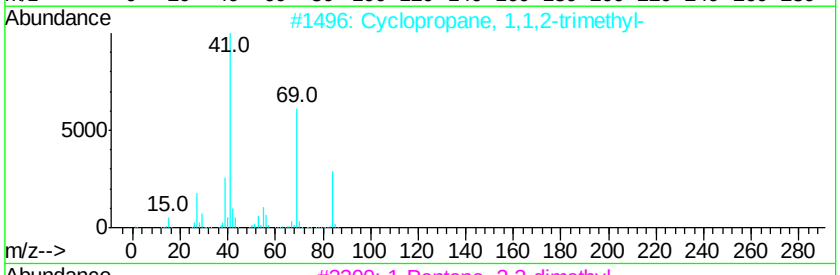
Peak Number 2 unknown4.85 Concentration Rank 7

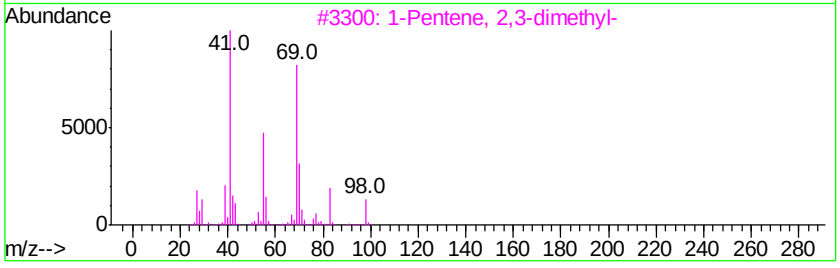
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	2.77 ng	173136	1,4-Dichlorobenzene-d4	6.88

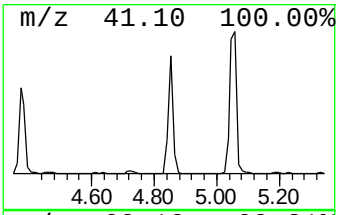
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	43
2	Cyclopropane, 1,1,2-trimethyl-	84	C6H12	004127-45-1	37
3	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	36
4	3-Penten-1-ol, 2-methyl-	100	C6H12O	062238-37-3	36
5	1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	25

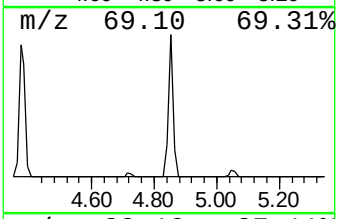


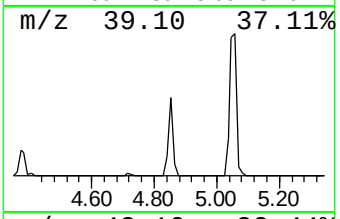


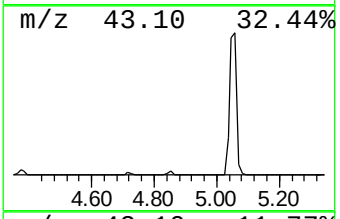


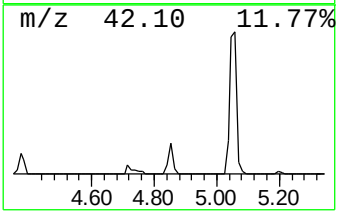












Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

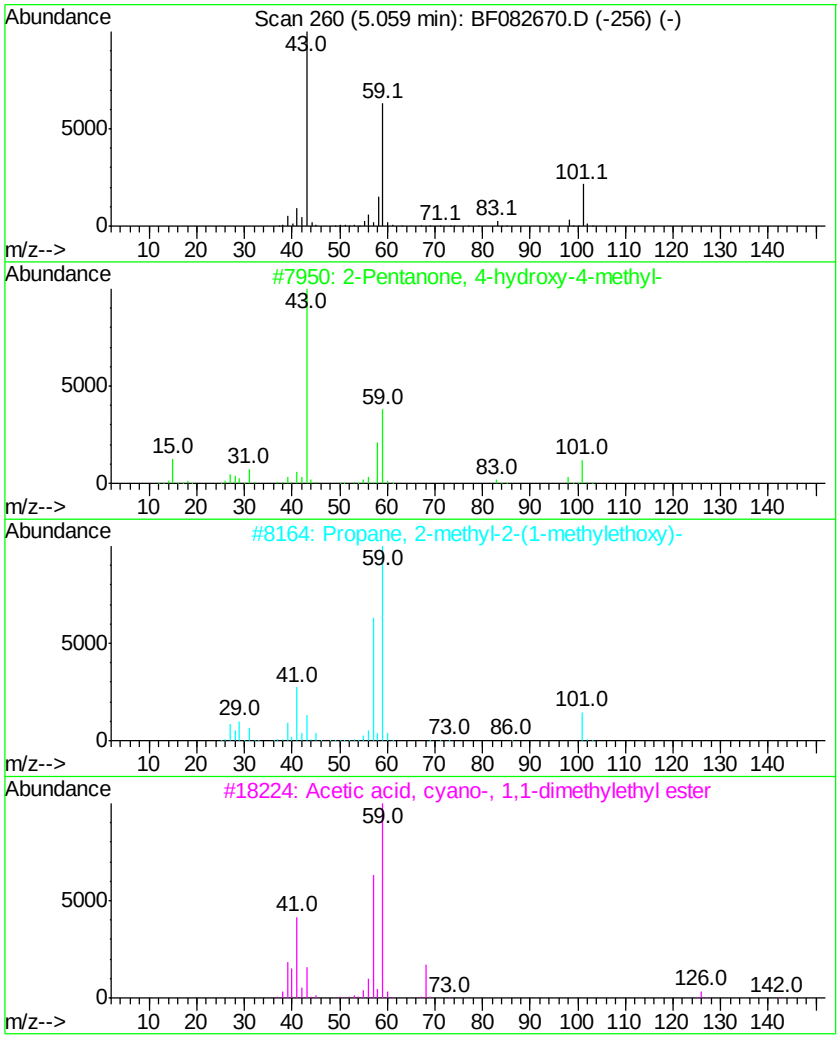
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

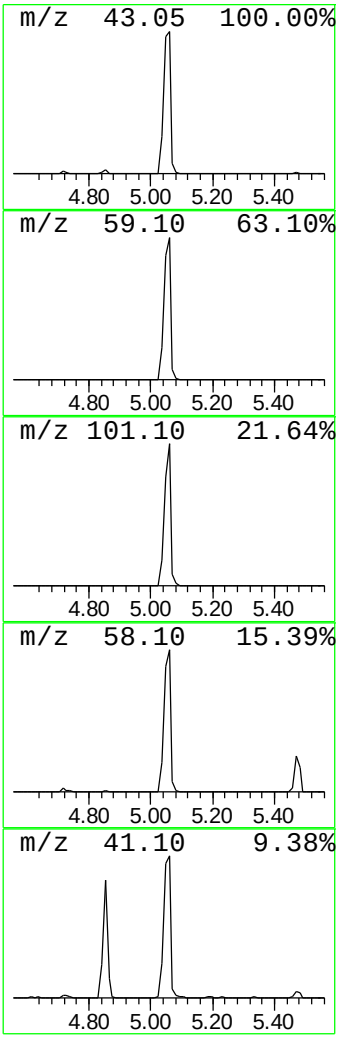
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	33.97 ng	2125850	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

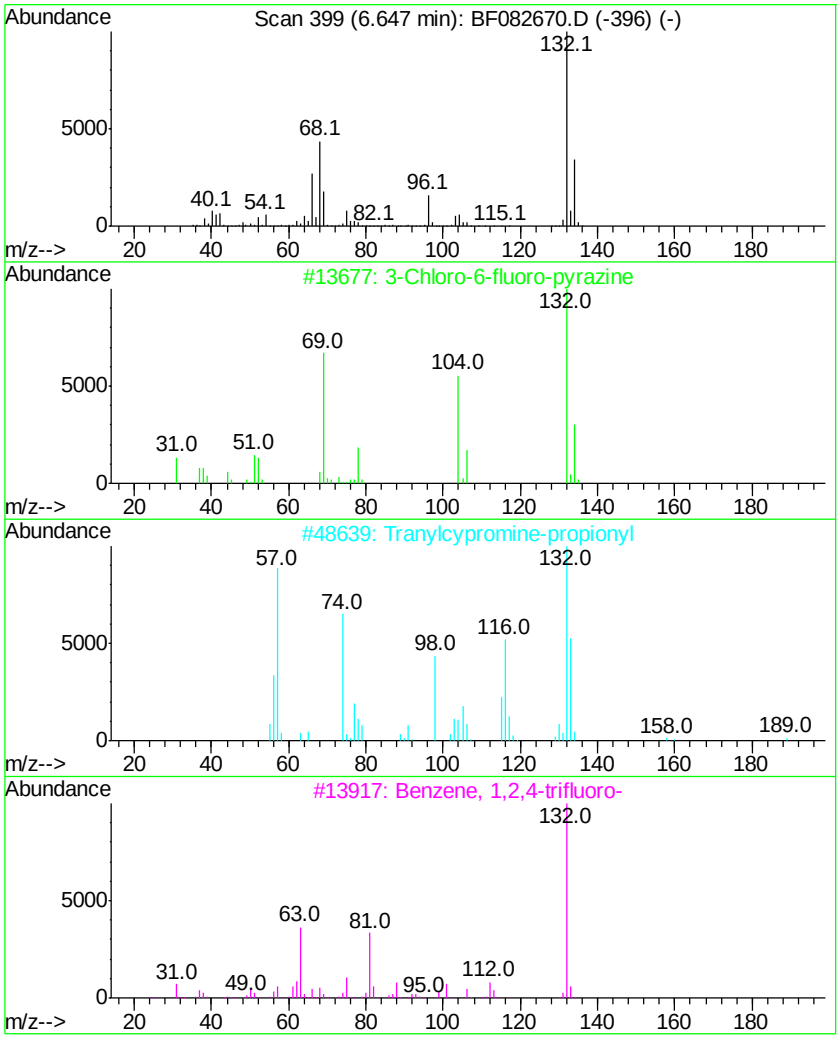
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

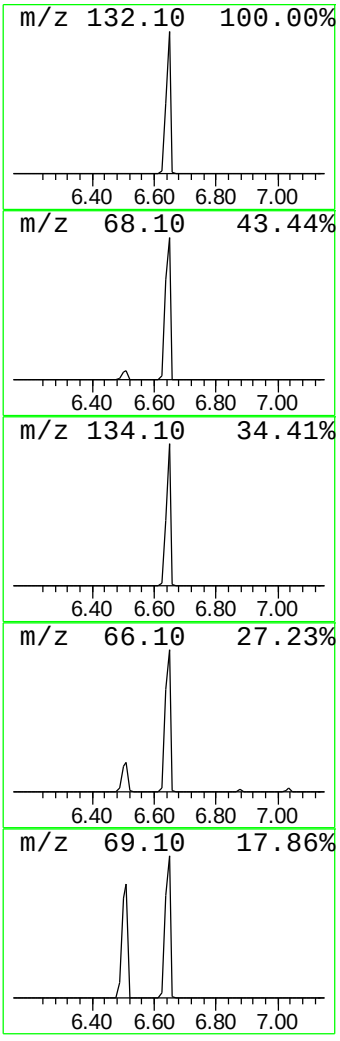
****

Peak Number 4 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	70.24 ng	4396150	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

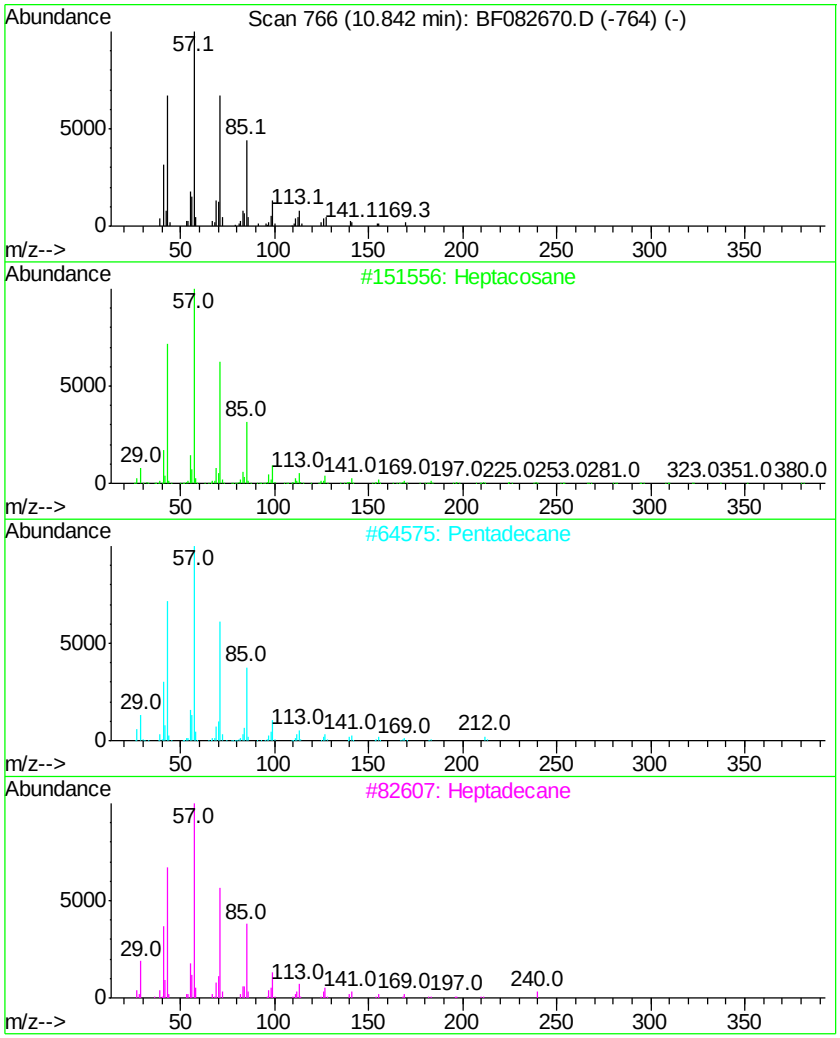
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

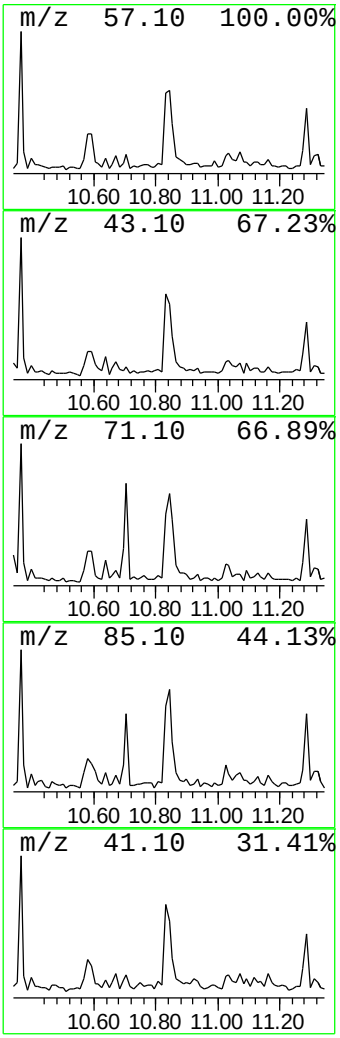
****

Peak Number 6 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	2.68 ng	254733	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
5	Hexadecane	226	C16H34	000544-76-3	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

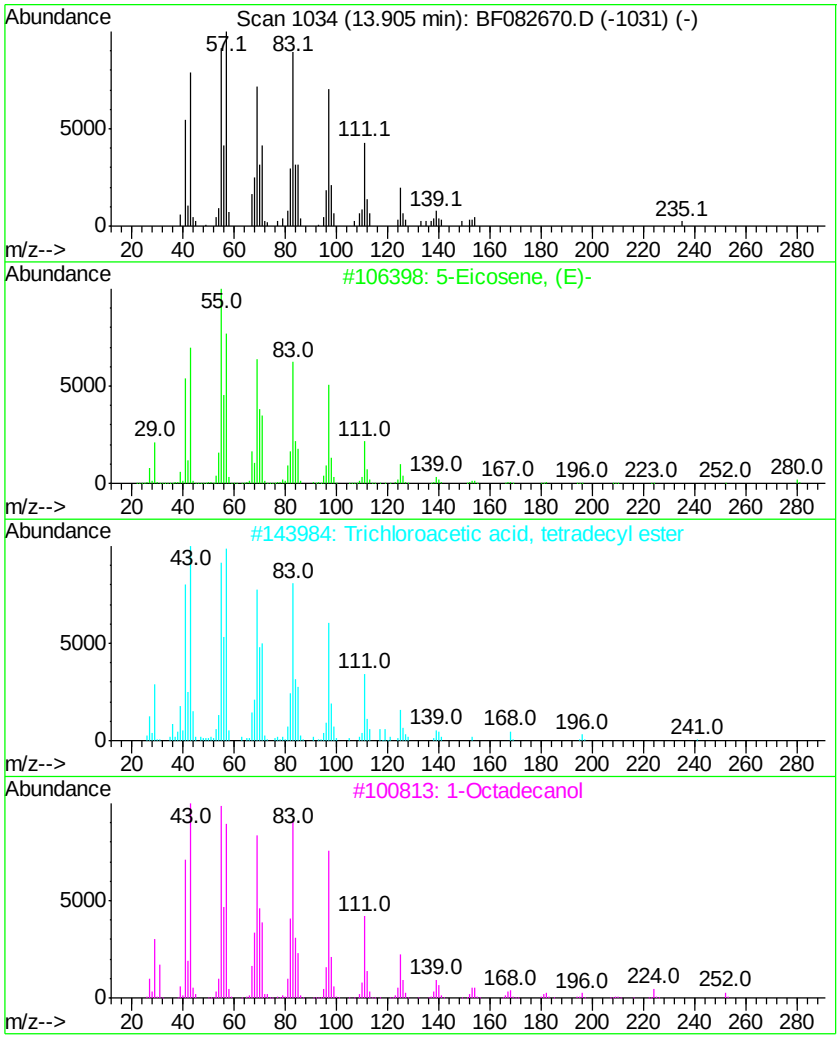
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

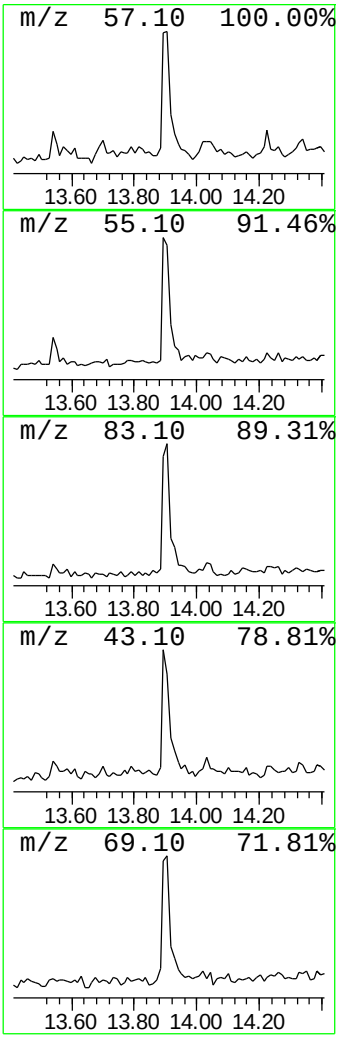
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	3.37 ng	258639	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	1-Octadecanol	270	C18H38O	000112-92-5	90
4	1-Eicosanol	298	C20H42O	000629-96-9	90
5	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

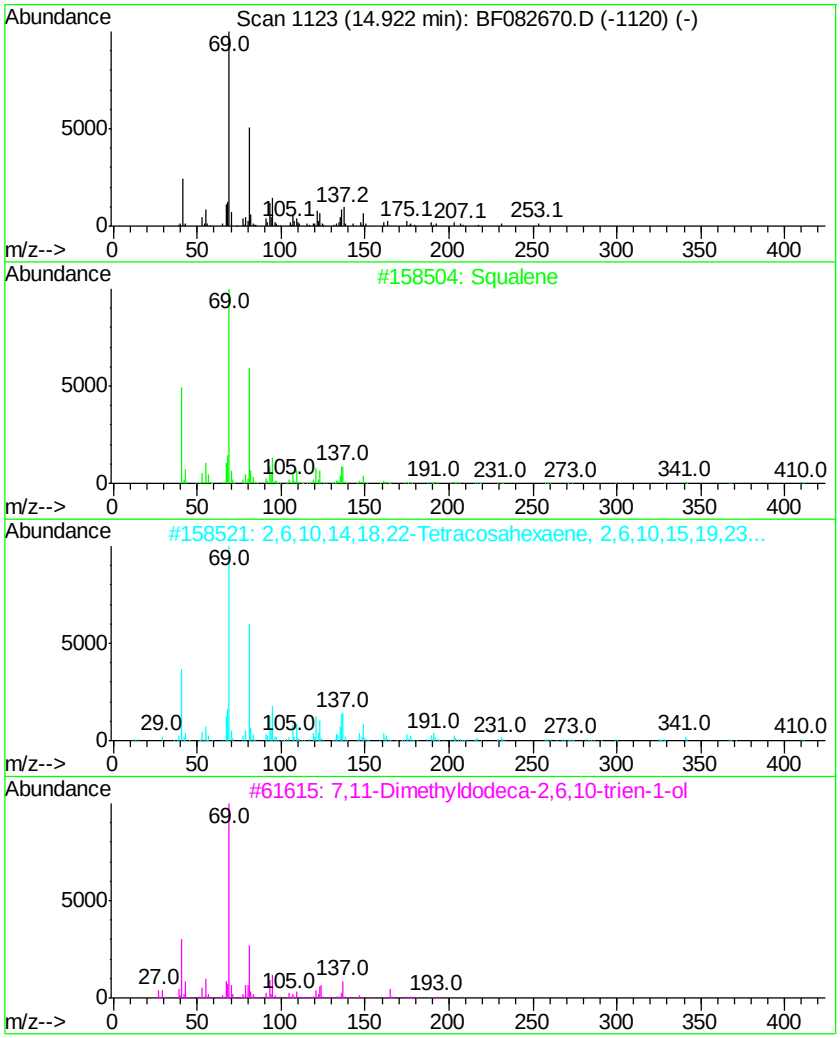
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

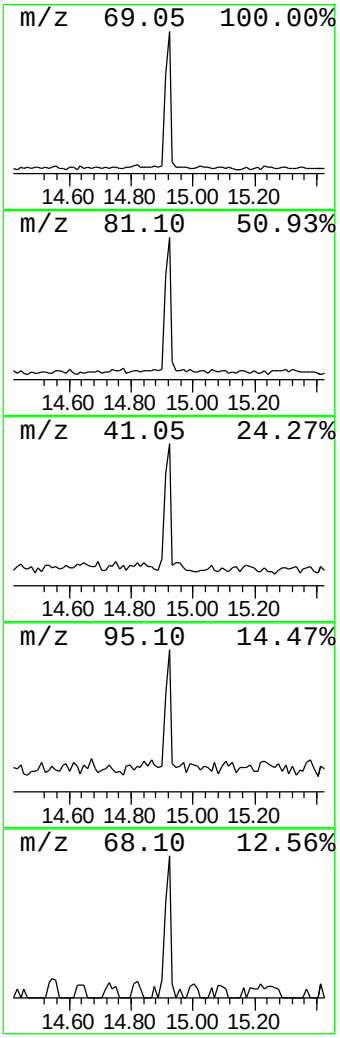
****

Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	3.15 ng	177528	Perylene-d12	15.49

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	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	87
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110315\
Data File : BF082670.D
Acq On : 3 Nov 2015 19:48
Operator : UM/IZ
Sample : G4242-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-5-20151102

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF103015.M
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
unknown4.37	4.37	3.6	ng	223904	1	6.88	1251690	20.0
unknown4.85	4.85	2.8	ng	173136	1	6.88	1251690	20.0
2-Pentanone, 4-hy...	5.06	34.0	ng	2125850	1	6.88	1251690	20.0
unknown6.65	6.65	70.2	ng	4396150	1	6.88	1251690	20.0
Heptacosane	10.84	2.7	ng	254733	4	11.40	1901640	20.0
5-Eicosene, (E)-	13.91	3.4	ng	258639	5	14.04	1535330	20.0
Squalene	14.92	3.1	ng	177528	6	15.49	1127280	20.0