LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\Data\BM033117\
Data File : BM009482.D
Acq On : 31 Mar 2017 20:10
Operator : SJ/MA
Sample : I2462-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-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:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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	4.969	316	320	327	rBV	68251	97348	1.32%	0.223%
2	5.422	390	397	410	rBV	1157155	1699036	22.98%	3.899%
3	7.004	659	666	678	rVB	662298	1049984	14.20%	2.409%
4	7.375	722	729	738	rBV	2233445	3500865	47.36%	8.034%
5	7.845	801	809	815	rBV	504688	775454	10.49%	1.779%
6	8.163	856	863	875	rVB	2101711	3465138	46.88%	7.952%
7	9.010	1000	1007	1017	rBV	1883273	3118373	42.19%	7.156%
8	10.645	1278	1285	1297	rVB	590858	1001714	13.55%	2.299%
9	13.110	1697	1704	1716	rBV	4302298	6312328	85.39%	14.485%
10	13.945	1840	1846	1851	rBV3	64614	95732	1.30%	0.220%
11	14.492	1931	1939	1946	rBV2	817611	1240229	16.78%	2.846%
12	15.980	2186	2192	2206	rBV	3504224	4842811	65.51%	11.113%
13	17.239	2399	2406	2414	rBV	1113349	1576644	21.33%	3.618%
14	17.604	2463	2468	2475	rBV	151294	228075	3.09%	0.523%
15	18.115	2549	2555	2565	rBV	196663	303684	4.11%	0.697%
16	18.539	2622	2627	2632	rVB2	88548	105437	1.43%	0.242%
17	18.974	2696	2701	2709	rBV2	255897	384505	5.20%	0.882%
18	19.392	2768	2772	2778	rBV2	124329	176330	2.39%	0.405%
19	19.656	2813	2817	2823	rVB3	79099	119417	1.62%	0.274%
20	19.856	2845	2851	2857	rBV	6260926	7391940	100.00%	16.963%
21	20.639	2980	2984	2988	rBV5	59813	76349	1.03%	0.175%
22	21.109	3060	3064	3069	rBV	214020	264869	3.58%	0.608%
23	21.315	3095	3099	3104	rBV2	104444	131101	1.77%	0.301%
24	21.415	3111	3116	3123	rBV	1772917	2194869	29.69%	5.037%
25	22.262	3256	3260	3264	rVB2	170345	205830	2.78%	0.472%
26	22.597	3313	3317	3325	rVB	827609	1090052	14.75%	2.501%
27	23.739	3504	3511	3520	rVB	1112976	2129466	28.81%	4.887%

Sum of corrected areas: 43577580

LSC Report - Integrated Chromatogram

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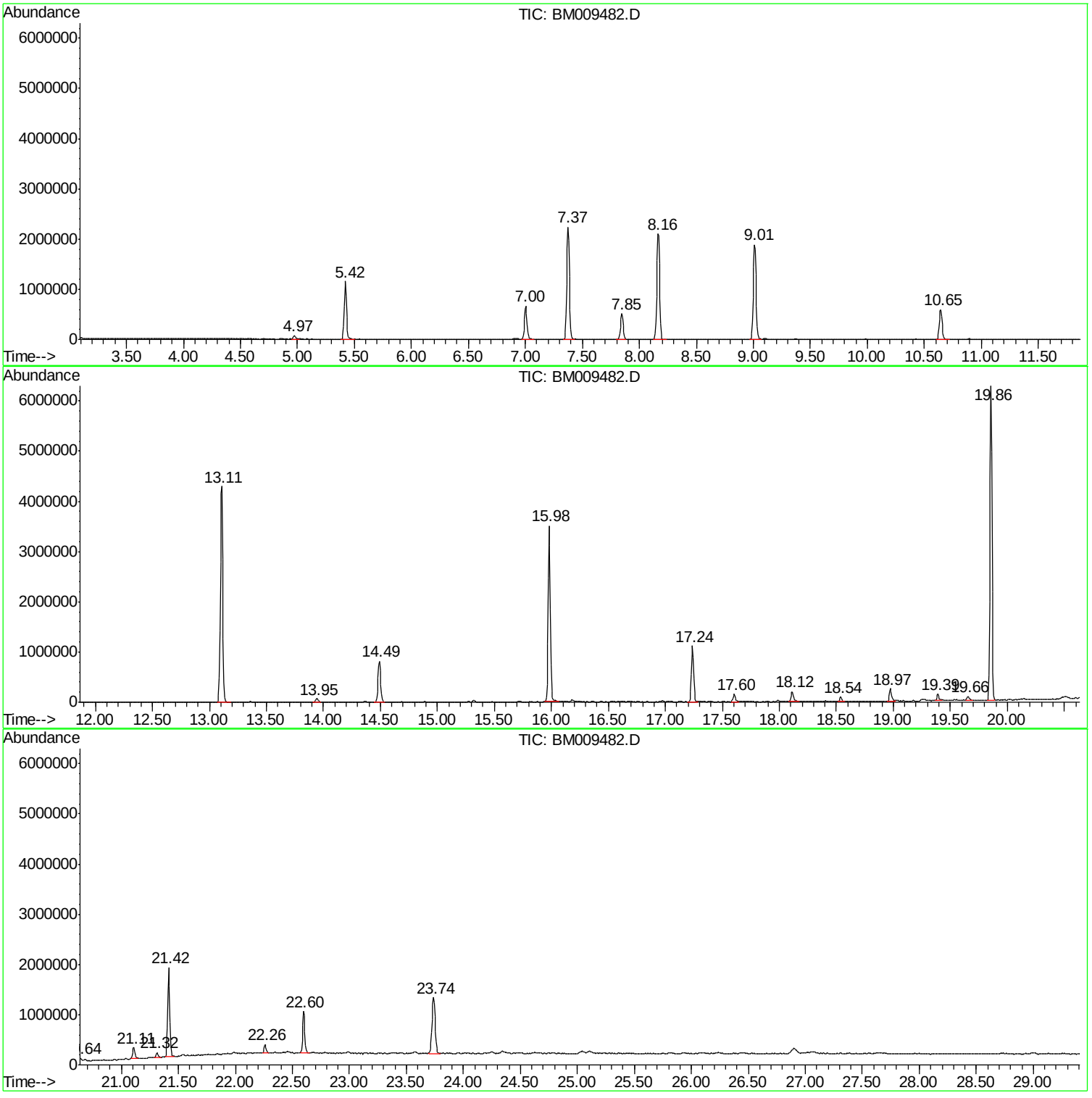
Data File : BM009482.D
Acq On : 31 Mar 2017 20:10
Operator : SJ/MA
Sample : I2462-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA M\Data\BM033117\
Data File : BM009482.D
Acq On : 31 Mar 2017 20:10
Operator : SJ/MA
Sample : I2462-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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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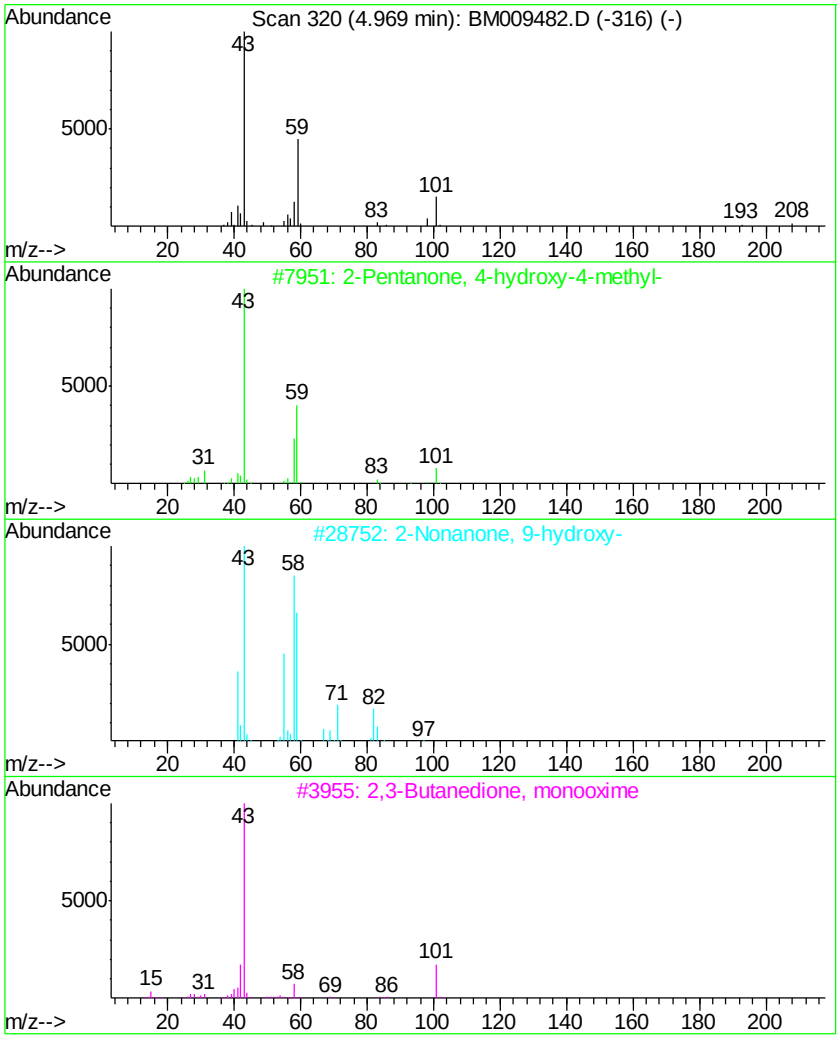
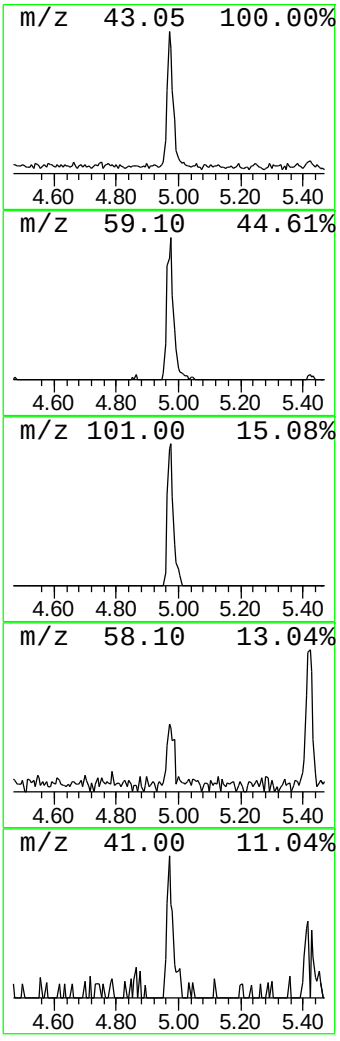
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	2.51 ng	97348	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5	Butane	58	C4H10	000106-97-8	9





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Acq On : 31 Mar 2017 20:10
Operator : SJ/MA
Sample : I2462-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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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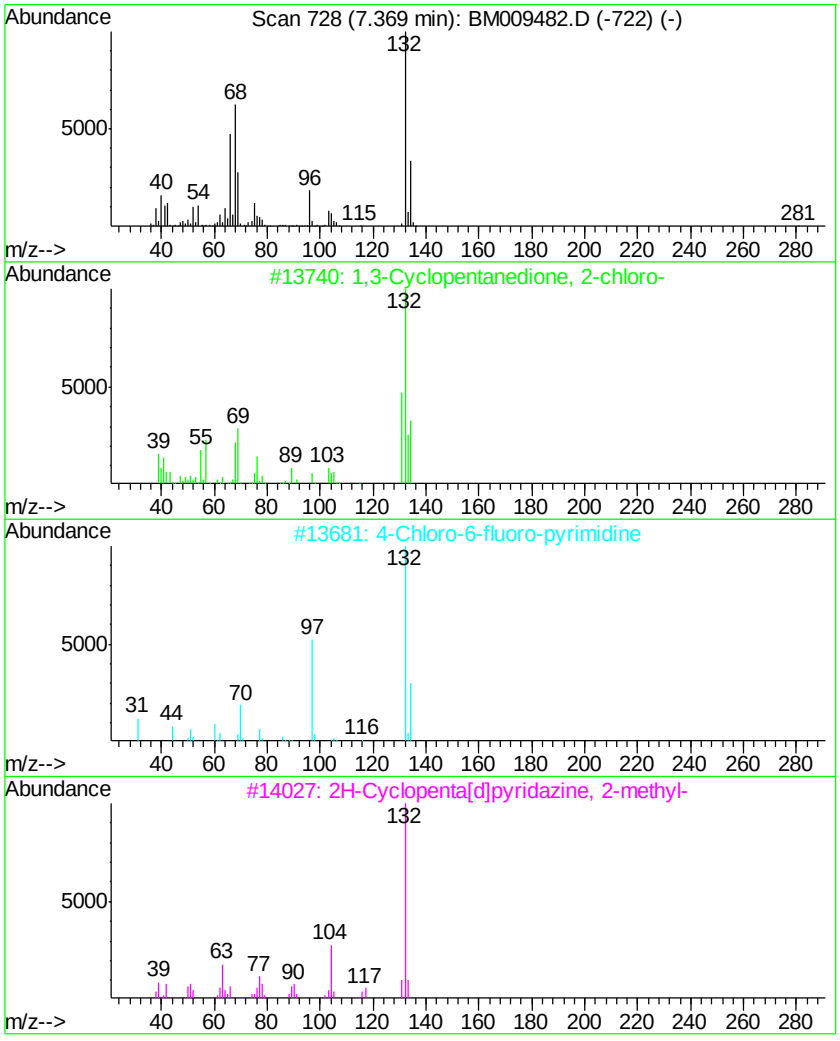
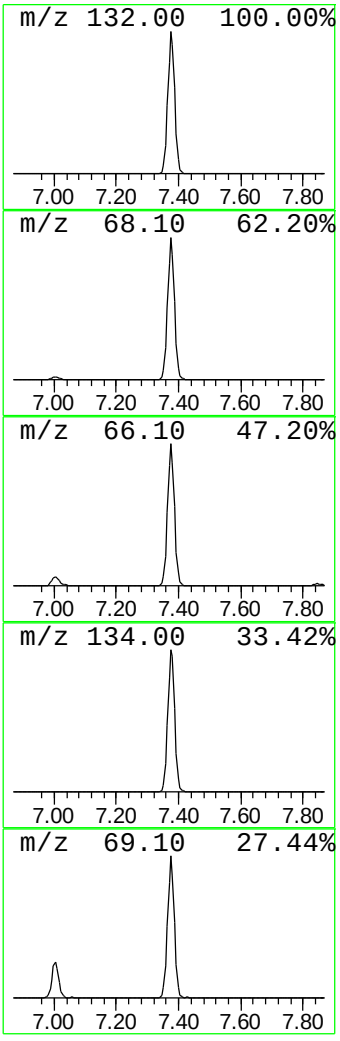
Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	90.29 ng	3500870	1,4-Dichlorobenzene-d4	7.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\Data\BM033117\
Data File : BM009482.D
Acq On : 31 Mar 2017 20:10
Operator : SJ/MA
Sample : I2462-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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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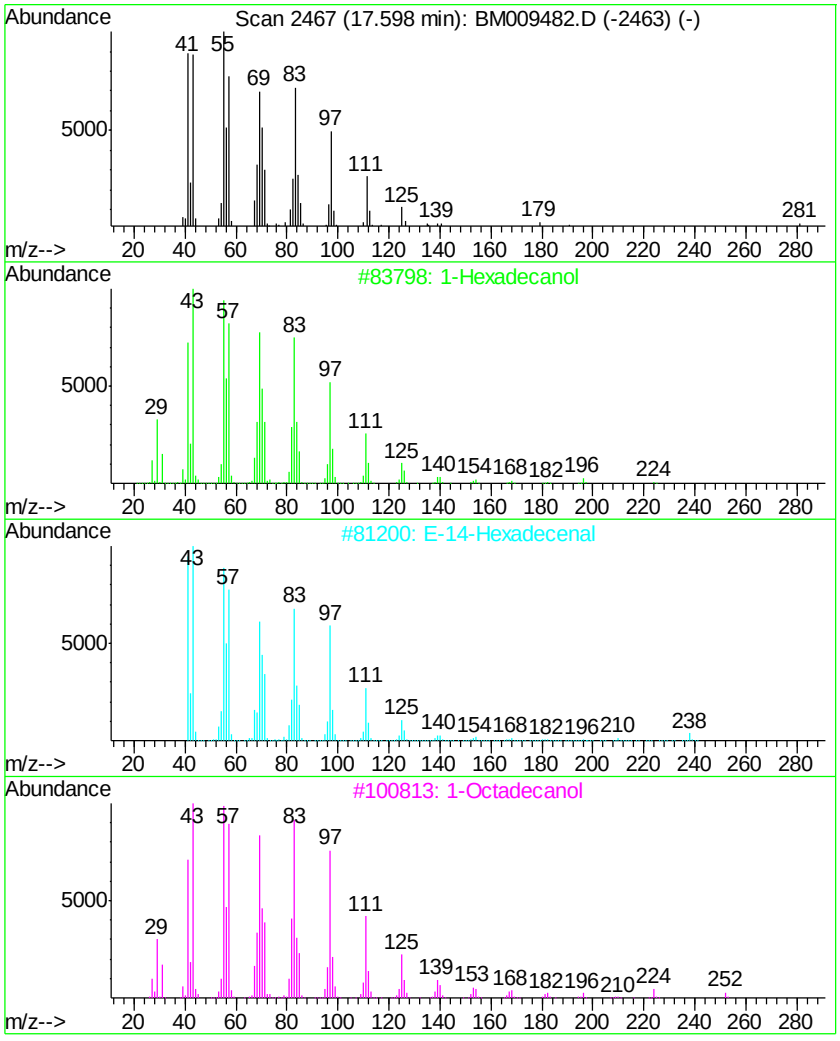
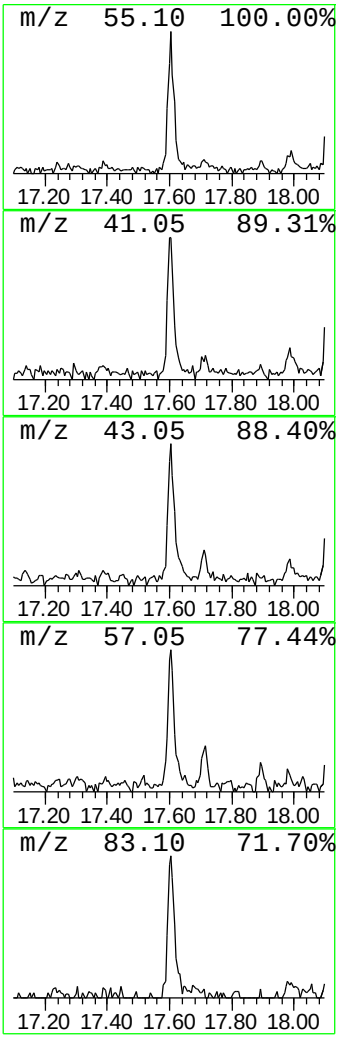
Peak Number 4 1-Hexadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.60	2.89 ng	228075	Phenanthrene-d10	17.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	91
3	1-Octadecanol	270	C18H38O	000112-92-5	91
4	Cyclotetradecane	196	C14H28	000295-17-0	91
5	3-Octadecene, (E)-	252	C18H36	007206-19-1	91





Data Path : Z:\HPCHEM1\BNA M\Data\BM033117\
Data File : BM009482.D
Acq On : 31 Mar 2017 20:10
Operator : SJ/MA
Sample : I2462-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.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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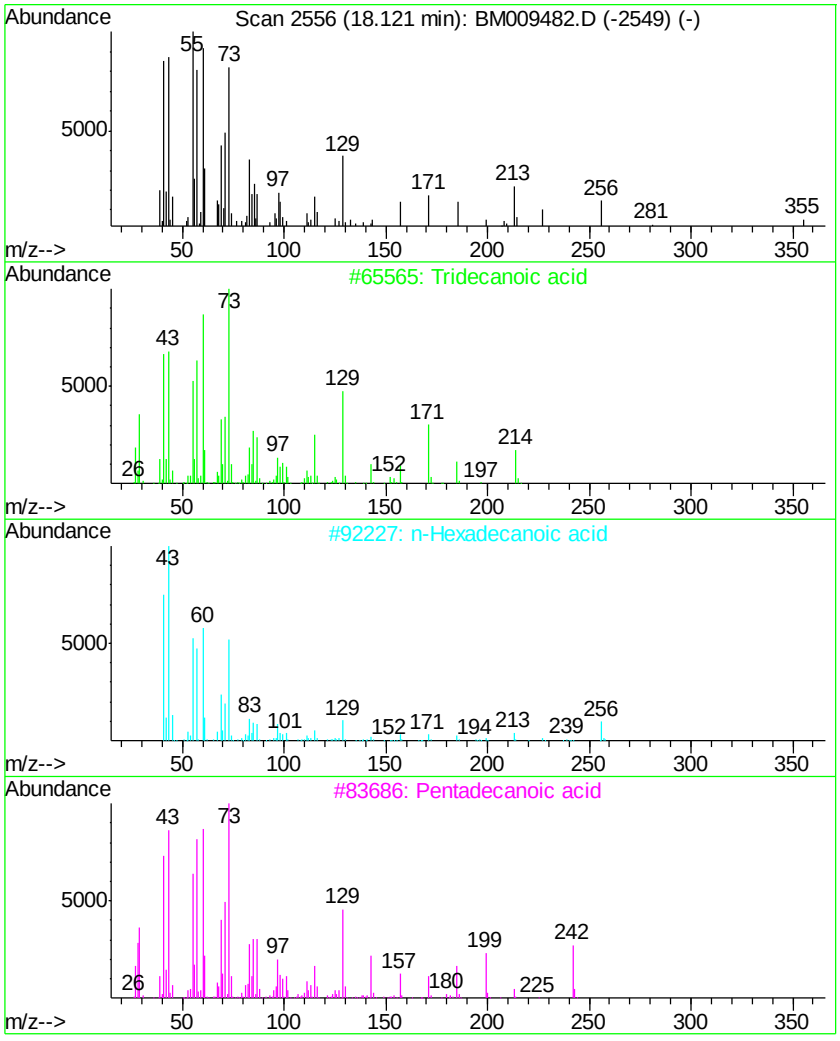
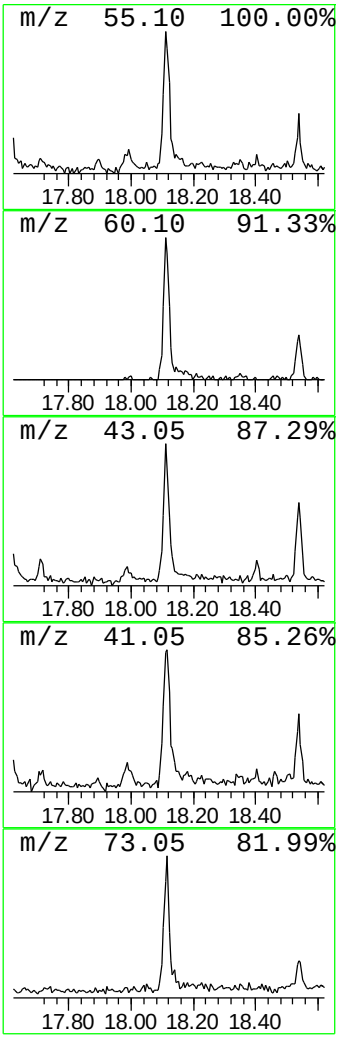
Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.12	3.85 ng	303684	Phenanthrene-d10	17.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\HPCHEM1\BNA M\Data\BM033117\
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Sample : I2462-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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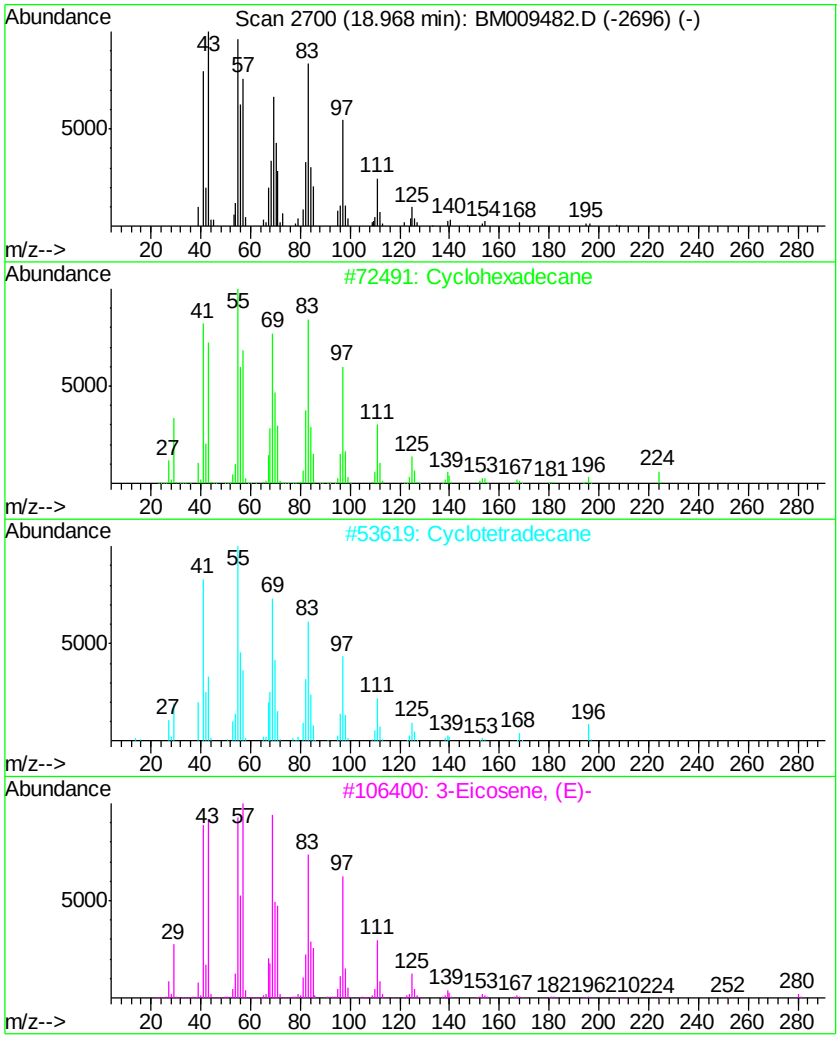
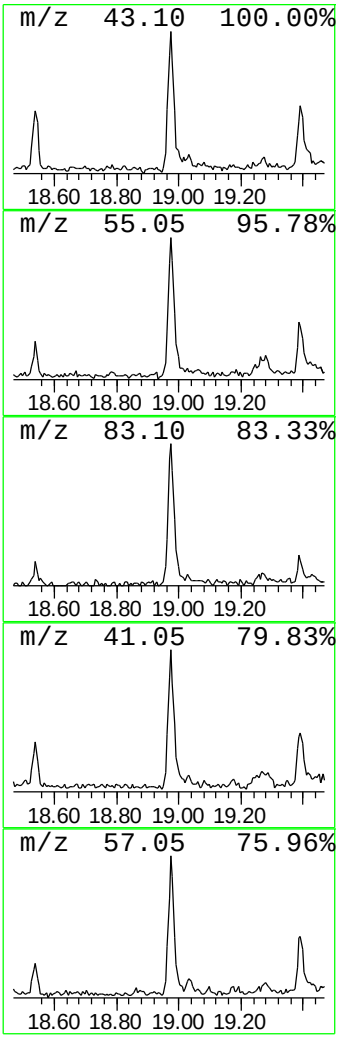
****

Peak Number 6 Cyclohexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.97	4.88 ng	384505	Phenanthrene-d10	17.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	97
2	Cyclotetradecane	196	C14H28	000295-17-0	95
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	94
5	1-Hexadecanol	242	C16H34O	036653-82-4	91





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Misc :
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Instrument : BNA_M
ClientSampleId : MW-3

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

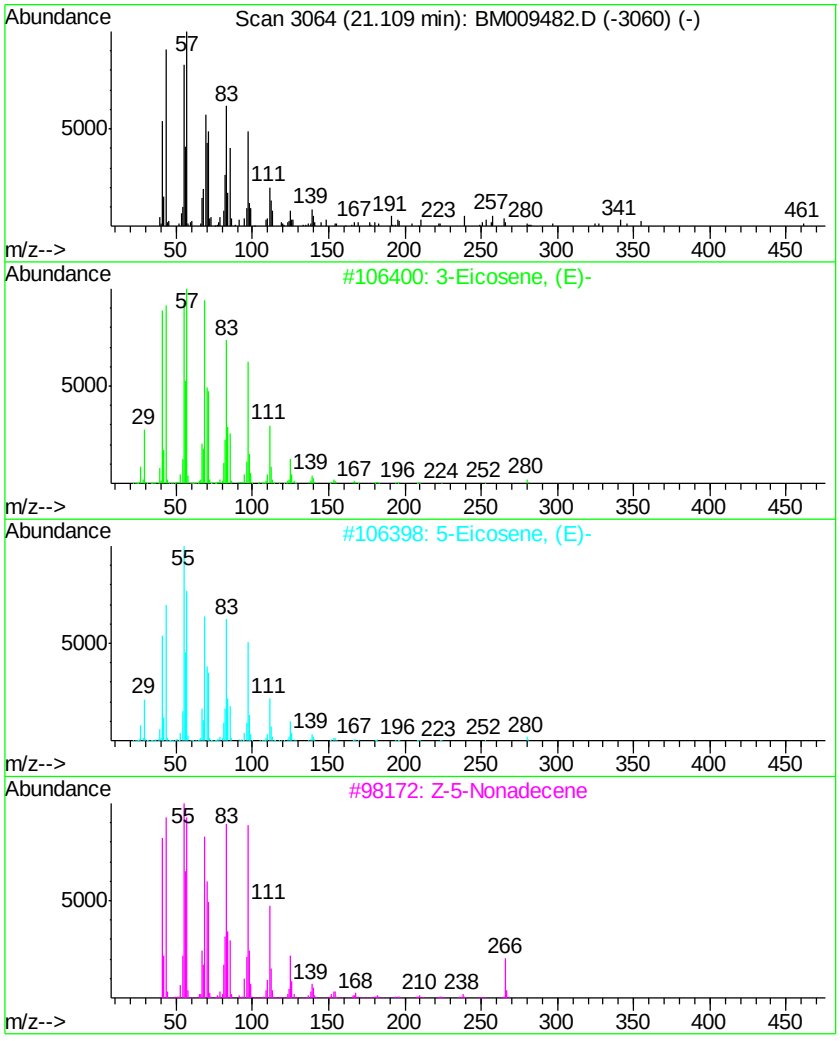
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

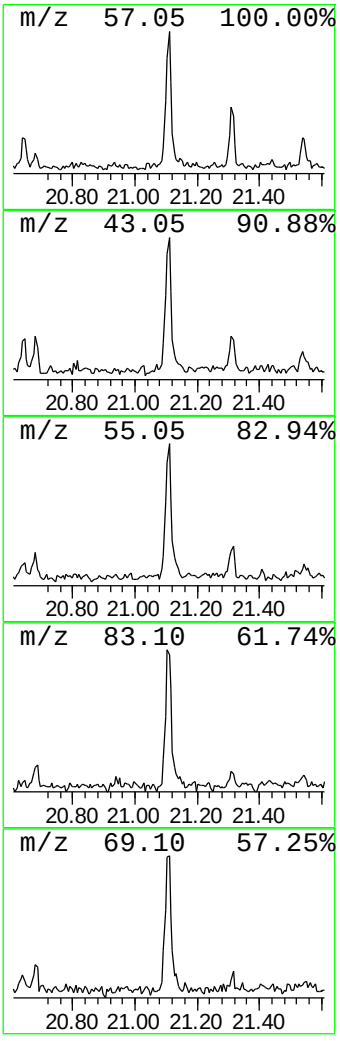
****

Peak Number 7 3-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.11	2.41 ng	264869	Chrysene-d12	21.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
3	Z-5-Nonadecene	266	C19H38	1000131-11-8	95
4	1-Nonadecene	266	C19H38	018435-45-5	94
5	Cyclotetradecane	196	C14H28	000295-17-0	92





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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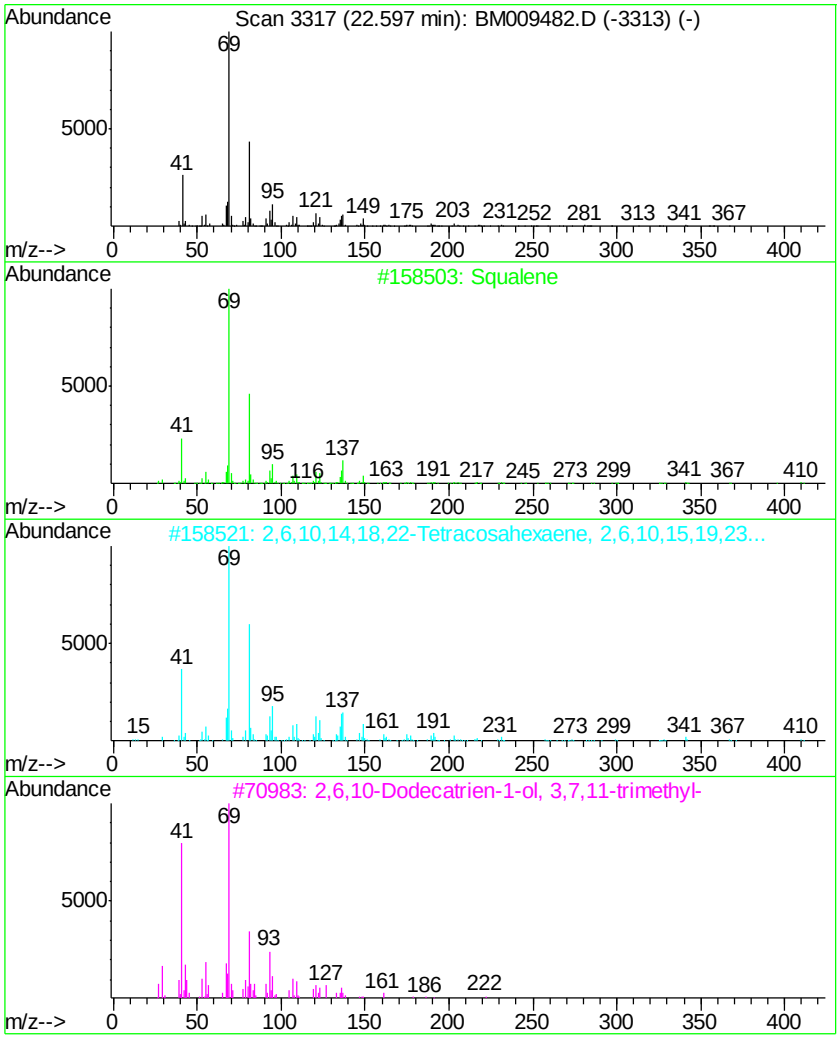
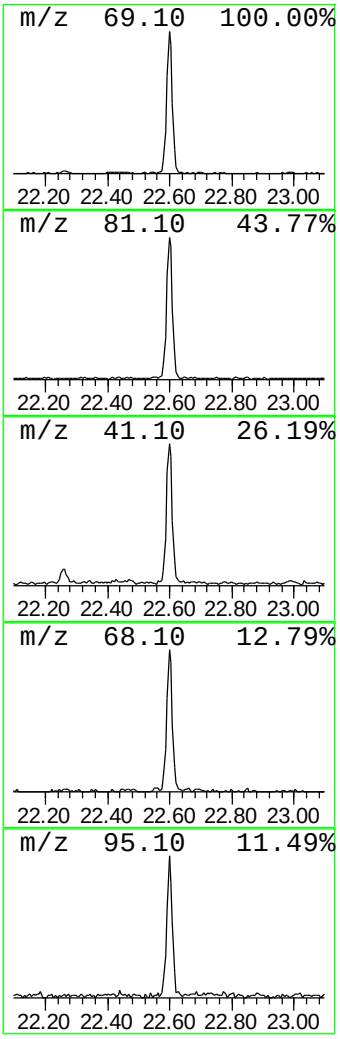
Peak Number 8 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.60	10.24 ng	1090050	Perylene-d12	23.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	90
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	83
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	78
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78





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
2-Pentanone, 4-hy...	4.97	2.5	ng	97348	1	7.85	775454	20.0
unknown7.37	7.37	90.3	ng	3500870	1	7.85	775454	20.0
1-Hexadecanol	17.60	2.9	ng	228075	4	17.24	1576640	20.0
Tridecanoic acid	18.12	3.9	ng	303684	4	17.24	1576640	20.0
Cyclohexadecane	18.97	4.9	ng	384505	4	17.24	1576640	20.0
3-Eicosene, (E)-	21.11	2.4	ng	264869	5	21.42	2194870	20.0
Squalene	22.60	10.2	ng	1090050	6	23.74	2129470	20.0