LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050318\
Data File : BF105091.D
Acq On : 3 May 2018 23:40
Operator : JU/SJ
Sample : J2709-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAYNE

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-BF040618.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	5.010	493	497	511	rBV	60285	119234	3.81%	0.481%
2	5.410	561	565	598	rBV	2072452	2878677	91.98%	11.601%
3	6.440	735	740	756	rBV	2109683	2855150	91.22%	11.506%
4	6.557	756	760	780	rVB	2744518	2974756	95.05%	11.988%
5	6.781	794	798	807	rBV	602636	607092	19.40%	2.447%
6	6.934	820	824	844	rBV	2257656	2352622	75.17%	9.481%
7	7.351	890	895	912	rBV	1507371	1780151	56.88%	7.174%
8	8.063	1013	1016	1039	rBV	761883	805596	25.74%	3.247%
9	9.145	1195	1200	1209	rBV	3037505	3129833	100.00%	12.613%
10	9.539	1263	1267	1274	rBV	253638	252210	8.06%	1.016%
11	9.739	1298	1301	1304	rBV	51369	39983	1.28%	0.161%
12	9.822	1311	1315	1324	rBV	871891	793508	25.35%	3.198%
13	10.239	1383	1386	1389	rVB	77024	54450	1.74%	0.219%
14	10.616	1446	1450	1461	rBV	1484969	1576338	50.36%	6.353%
15	10.710	1464	1466	1472	rVB	53064	58035	1.85%	0.234%
16	11.310	1565	1568	1577	rBV	632899	637647	20.37%	2.570%
17	11.839	1654	1658	1668	rBV	342491	371170	11.86%	1.496%
18	12.622	1787	1791	1798	rBV	95932	111550	3.56%	0.450%
19	12.904	1834	1839	1843	rBV	2253489	2132076	68.12%	8.592%
20	13.827	1993	1996	2007	rBV2	78439	122993	3.93%	0.496%
21	14.016	2024	2028	2038	rBV	443629	506602	16.19%	2.042%
22	14.104	2039	2043	2047	rBV	71339	70499	2.25%	0.284%
23	14.851	2167	2170	2176	rBV6	25056	40854	1.31%	0.165%
24	14.933	2181	2184	2189	rVB	93264	102622	3.28%	0.414%
25	15.574	2288	2293	2305	rBV	294481	439853	14.05%	1.773%

Sum of corrected areas: 24813501

LSC Report - Integrated Chromatogram

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Misc :
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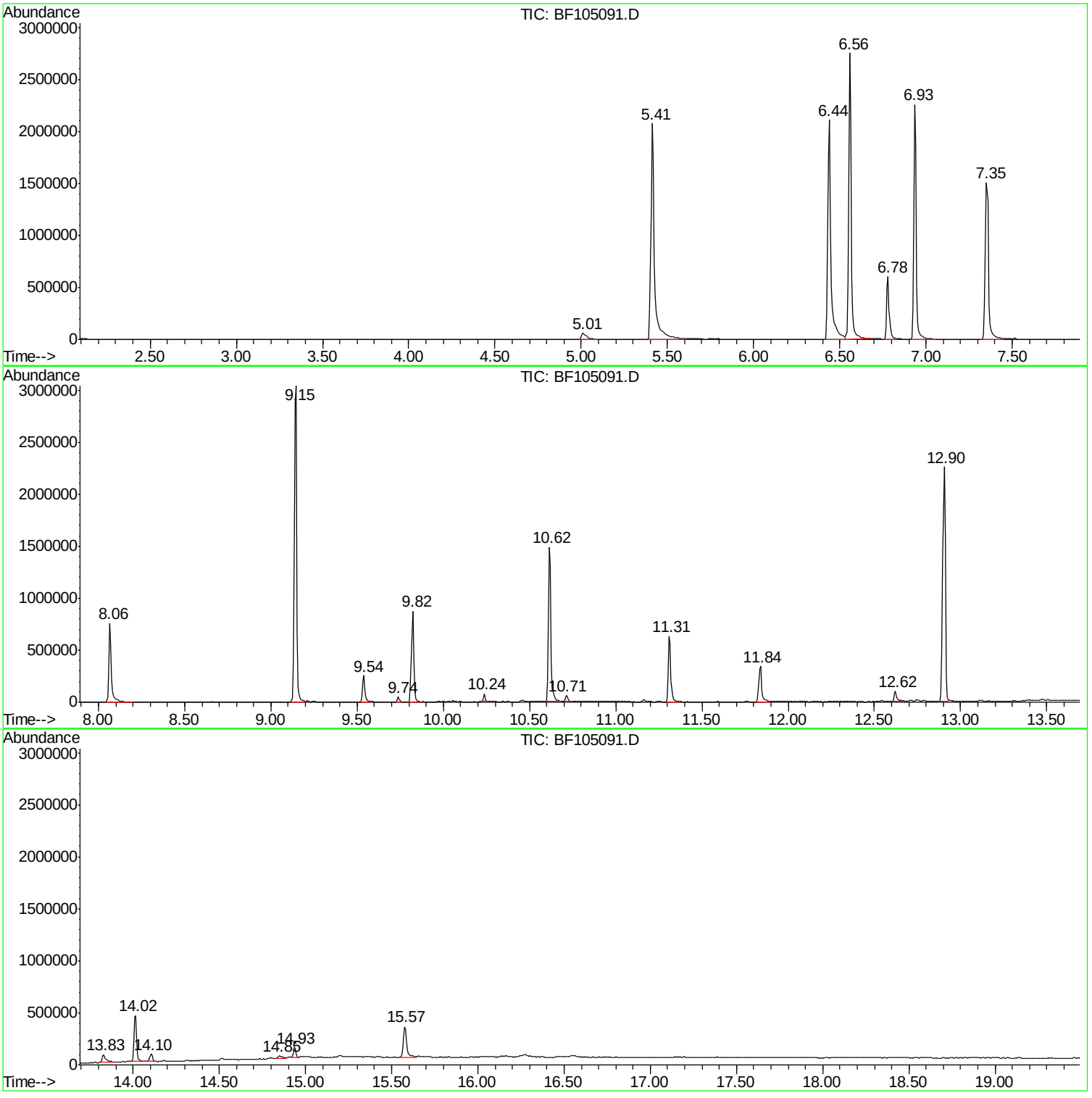
Instrument : BNA_F
ClientSampleId : WAYNE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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

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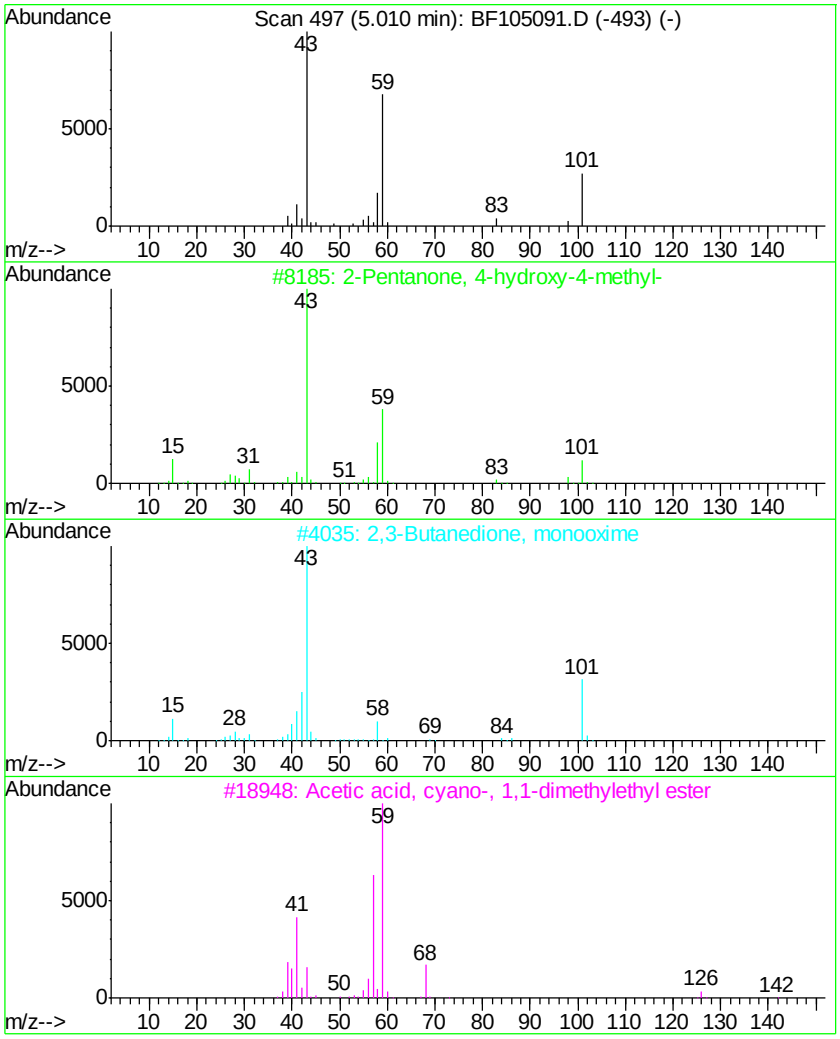
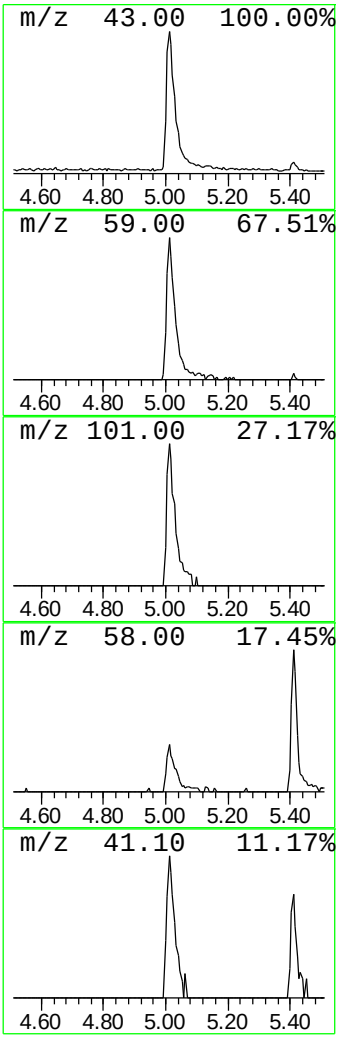
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	3.93 ng	119234	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9





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Instrument : BNA_F
ClientSampleId : WAYNE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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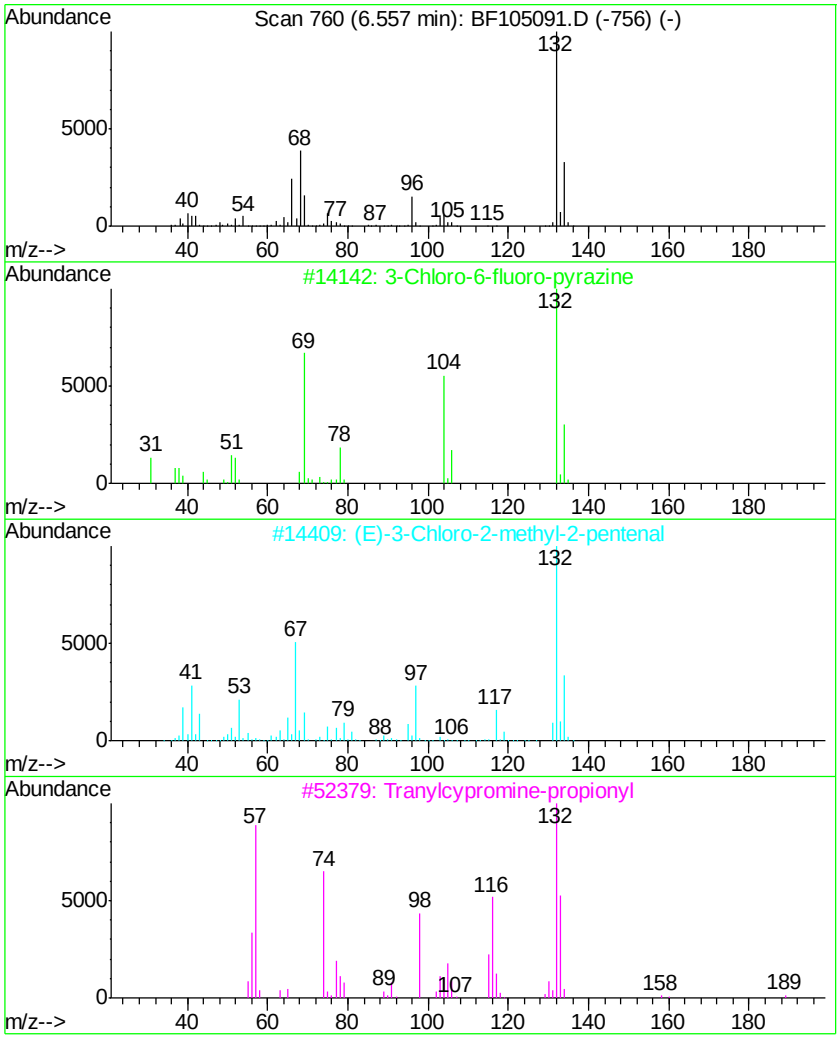
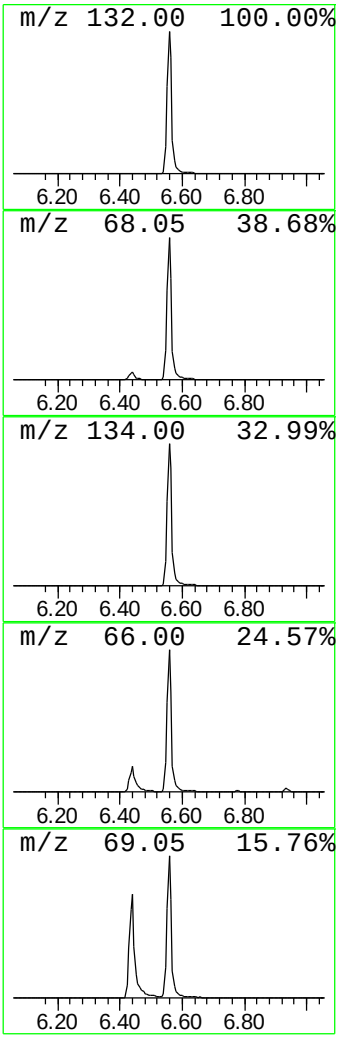
Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	98.00 ng	2974760	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Data File : BF105091.D
Acq On : 3 May 2018 23:40
Operator : JU/SJ
Sample : J2709-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAYNE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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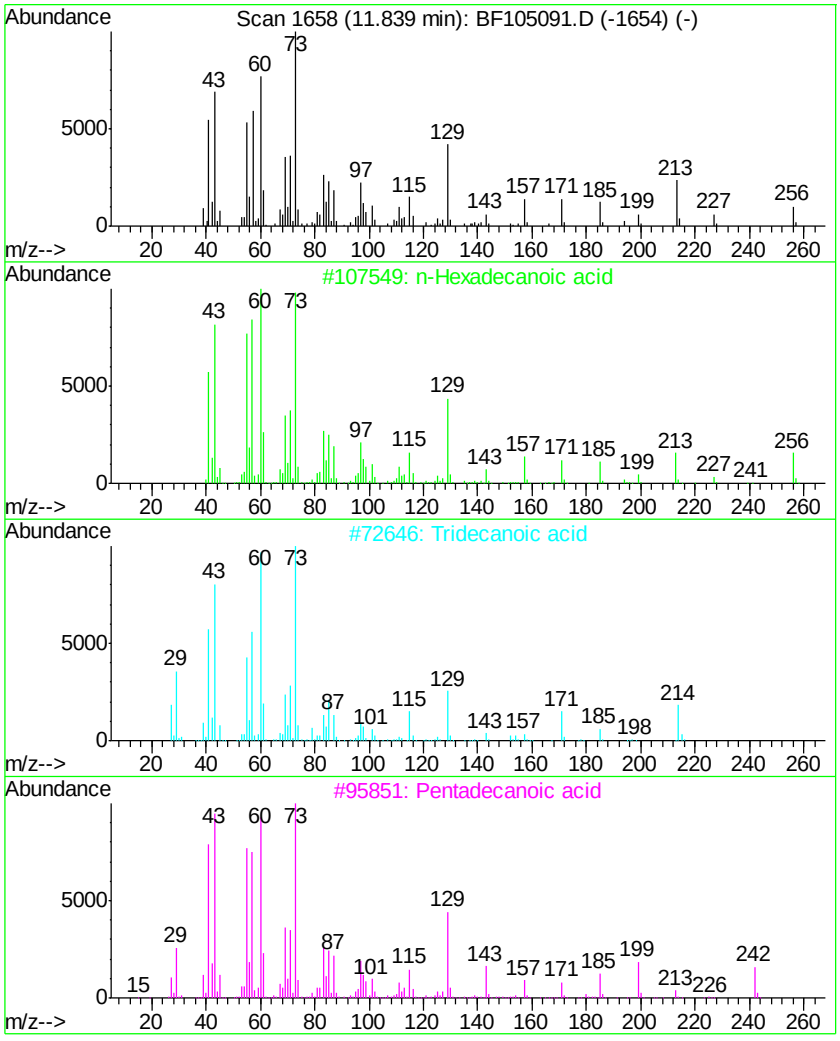
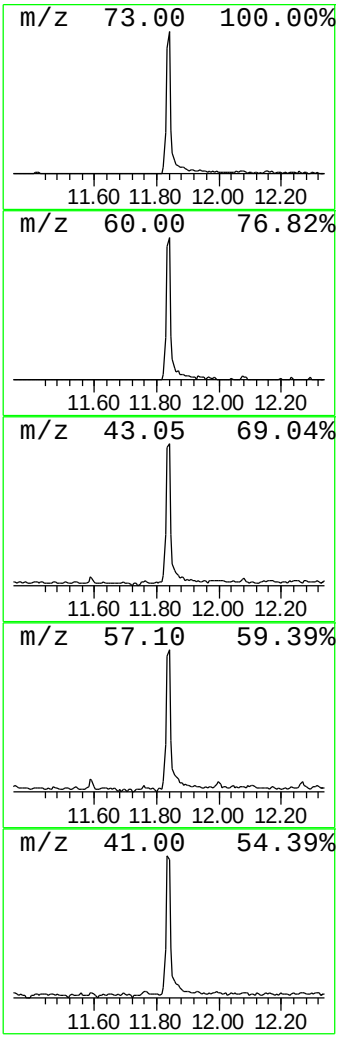
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	11.64 ng	371170	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Data File : BF105091.D
Acq On : 3 May 2018 23:40
Operator : JU/SJ
Sample : J2709-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAYNE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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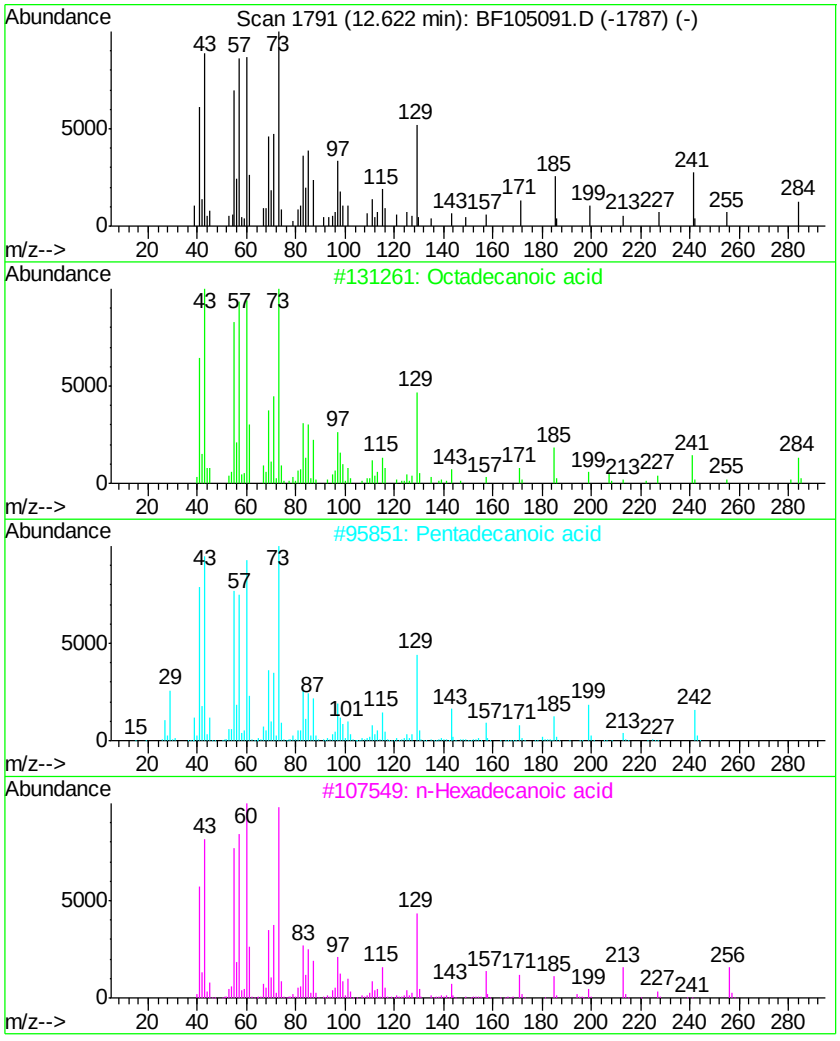
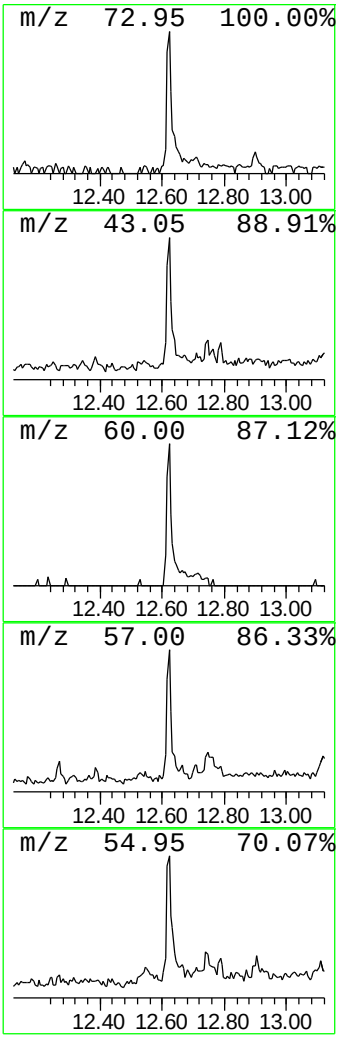
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	3.50 ng	111550	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050318\
Data File : BF105091.D
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Operator : JU/SJ
Sample : J2709-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WAYNE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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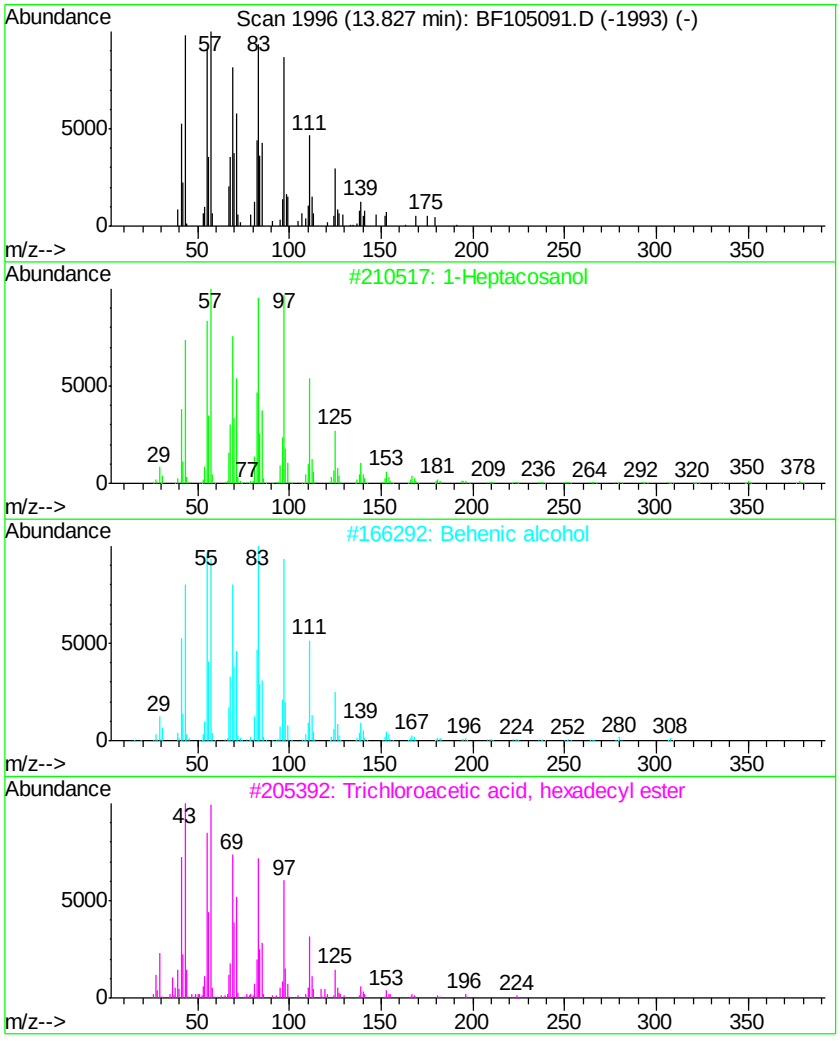
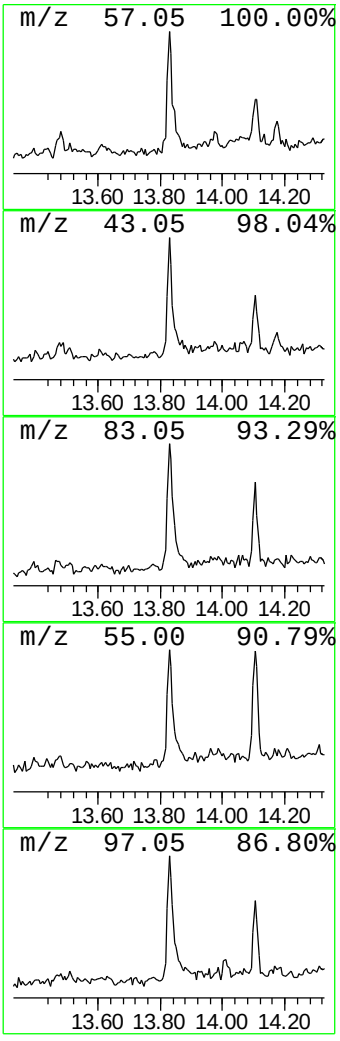
Peak Number 6 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.86 ng	122993	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Octacosanol	410	C28H58O	000557-61-9	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





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Instrument : BNA_F
ClientSampleId : WAYNE

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

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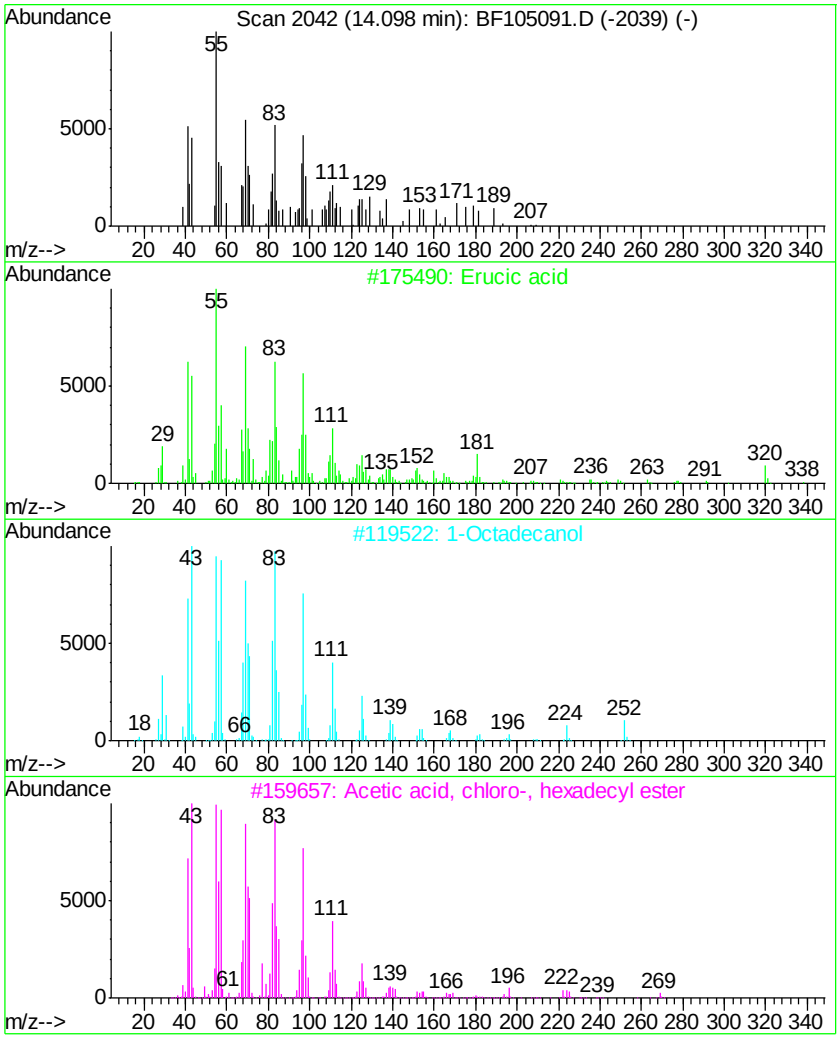
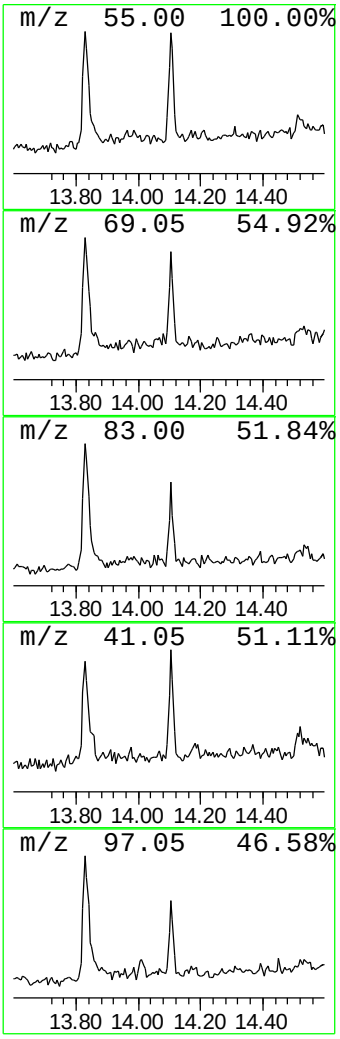
Peak Number 7 Erucic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	2.78 ng	70499	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Erucic acid	338	C22H42O2	000112-86-7	83
2	1-Octadecanol	270	C18H38O	000112-92-5	70
3	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	62
4	1-Hexadecanol	242	C16H34O	036653-82-4	62
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	62





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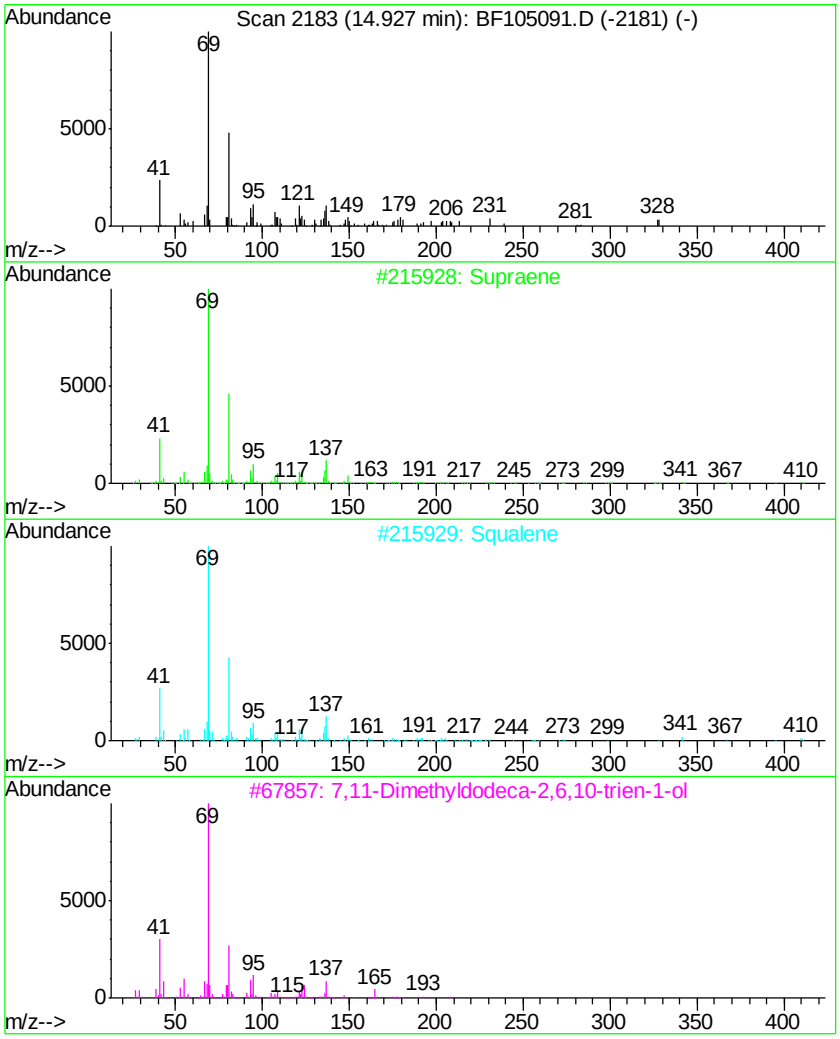
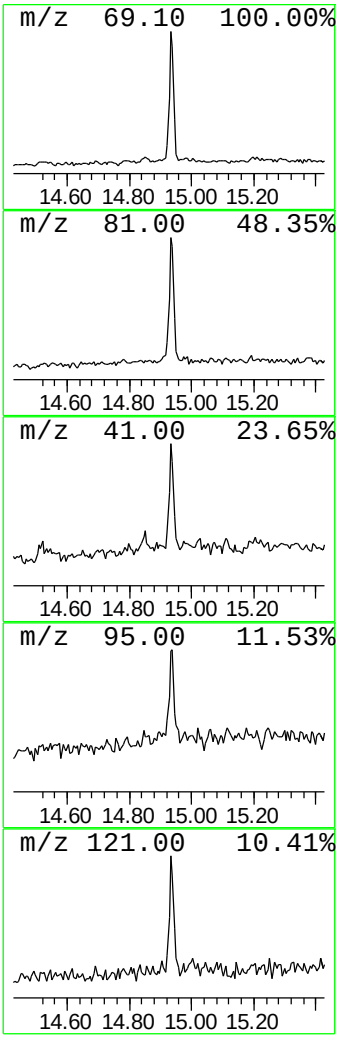
Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	4.67 ng	102622	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	Squalene	410	C30H50	000111-02-4	87
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
5	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72





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
2-Pentanone, 4-hy...	5.01	3.9	ng	119234	1	6.78	607092	20.0
unknown6.56	6.56	98.0	ng	2974760	1	6.78	607092	20.0
n-Hexadecanoic acid	11.84	11.6	ng	371170	4	11.31	637647	20.0
Octadecanoic acid	12.62	3.5	ng	111550	4	11.31	637647	20.0
1-Heptacosanol	13.83	4.9	ng	122993	5	14.02	506602	20.0
Erucic acid	14.10	2.8	ng	70499	5	14.02	506602	20.0
Supraene	14.93	4.7	ng	102622	6	15.57	439853	20.0