

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062818\
 Data File : BF106927.D
 Acq On : 28 Jun 2018 18:15
 Operator : JU/SJ
 Sample : PB110677BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB110677BL

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_F\METHODS\8270-BF061918.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	5.201	483	487	501	rBB	151707	197657	8.37%	1.169%
2	5.601	550	555	558	rBV	1724514	1642484	69.57%	9.713%
3	6.595	719	724	728	rBV	1503010	1666782	70.60%	9.857%
4	6.731	742	747	750	rBV	1843873	1703742	72.17%	10.075%
5	6.954	781	785	788	rBV	461750	405708	17.18%	2.399%
6	7.107	807	811	815	rBV	1534371	1403416	59.44%	8.299%
7	7.519	875	881	884	rBV	1108605	1102282	46.69%	6.518%
8	8.237	998	1003	1009	rBV	519757	514520	21.79%	3.043%
9	9.307	1180	1185	1189	rBV	2105524	2139157	90.61%	12.650%
10	9.995	1297	1302	1312	rBB	631958	607494	25.73%	3.592%
11	10.789	1432	1437	1440	rBV	1511754	1434804	60.77%	8.485%
12	11.489	1552	1556	1563	rBV	691256	658880	27.91%	3.896%
13	13.072	1820	1825	1828	rBV	2372822	2360870	100.00%	13.961%
14	14.136	2002	2006	2015	rBV	574196	581292	24.62%	3.437%
15	14.983	2146	2150	2154	rVB	46100	47909	2.03%	0.283%
16	15.677	2263	2268	2279	rVB	342802	443316	18.78%	2.622%

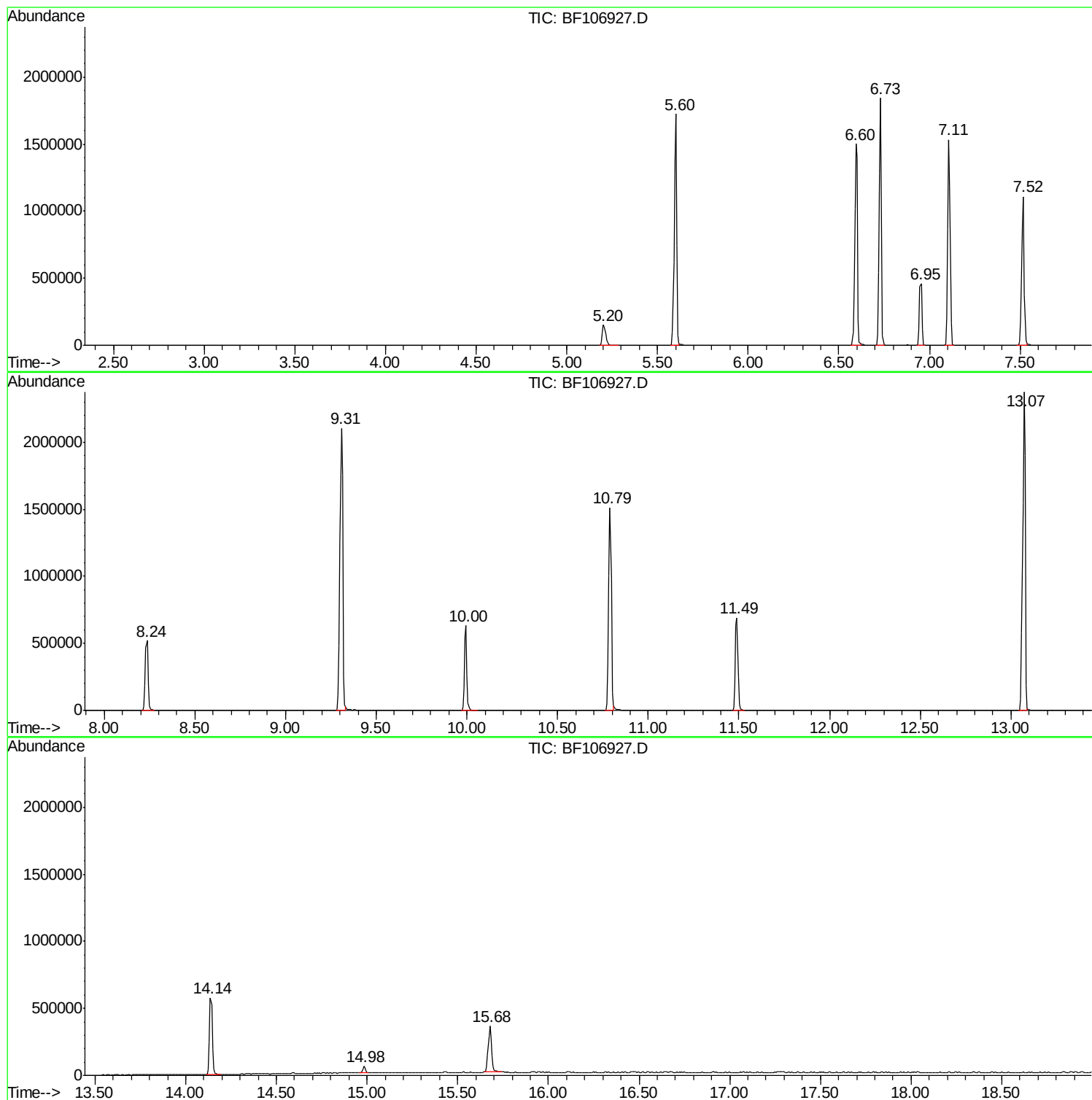
Sum of corrected areas: 16910313

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



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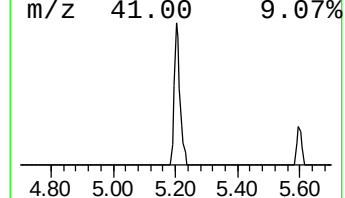
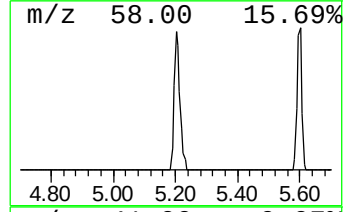
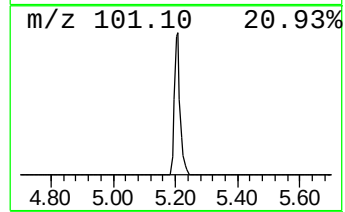
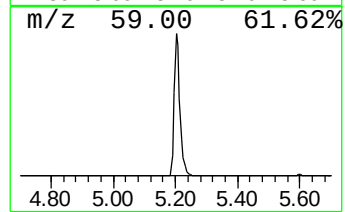
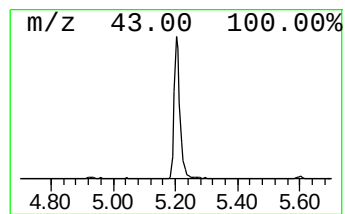
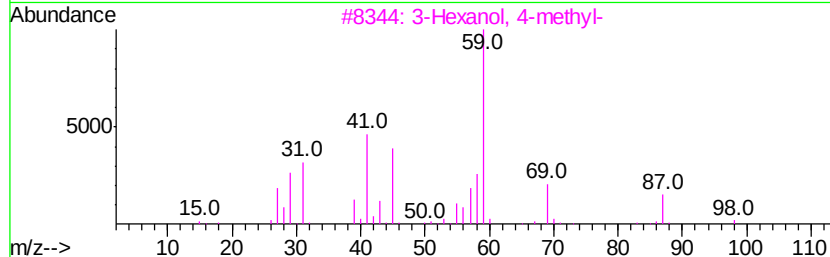
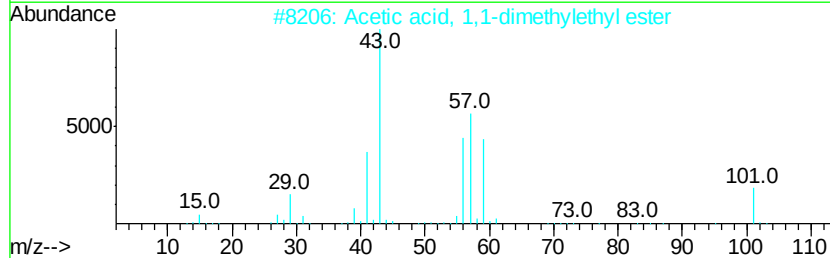
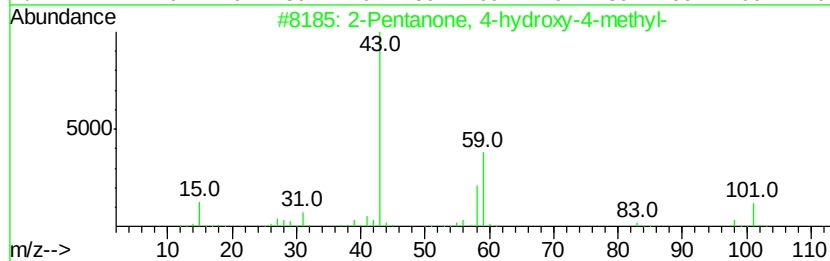
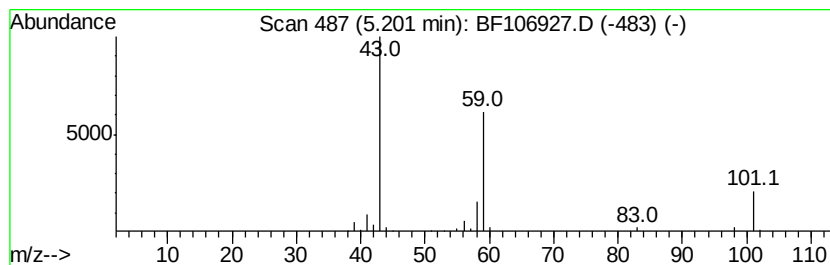
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	9.74 ng	197657	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
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			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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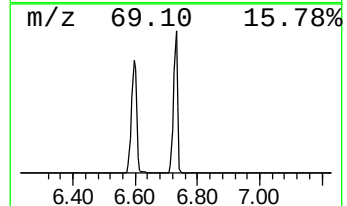
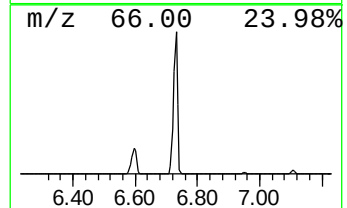
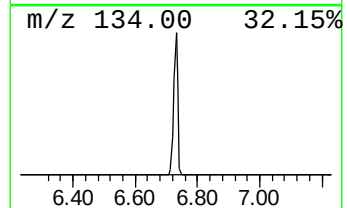
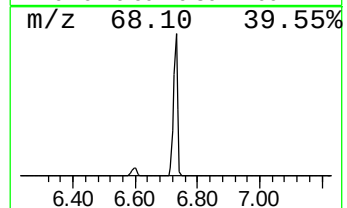
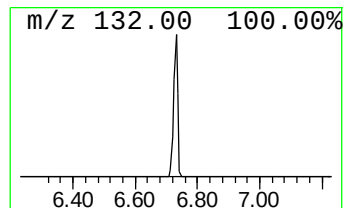
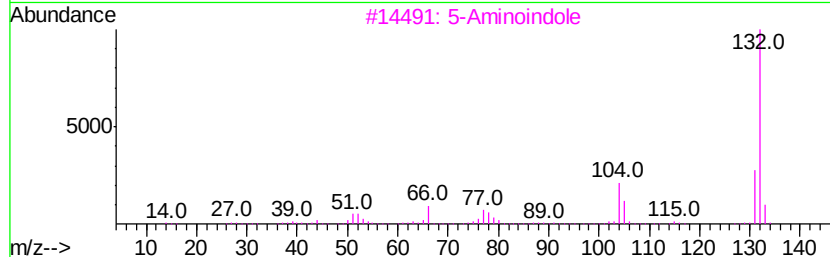
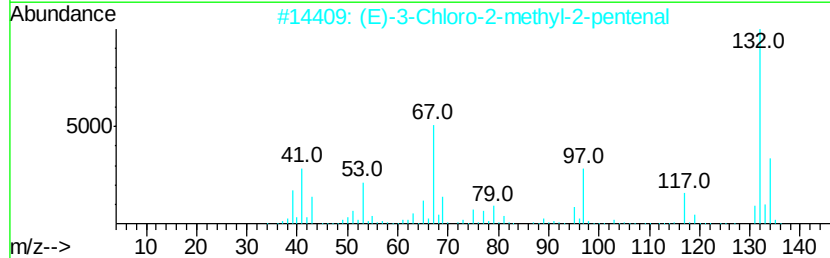
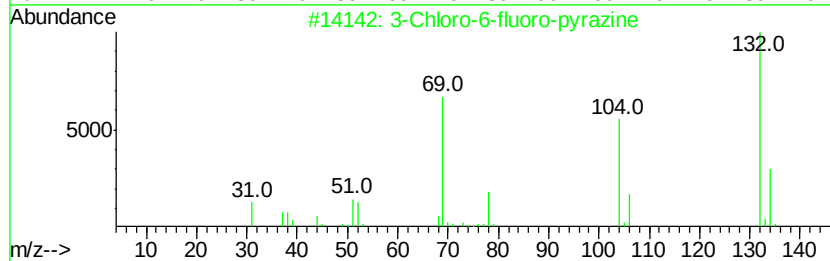
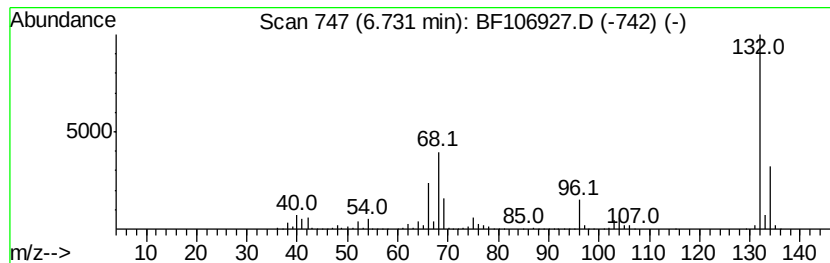
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	83.99 ng	1703740	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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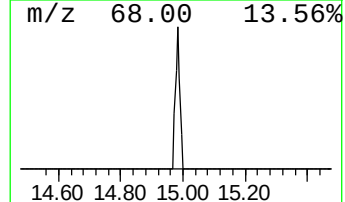
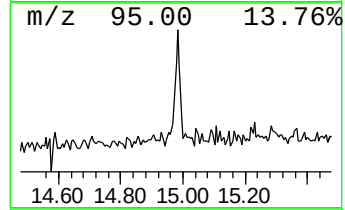
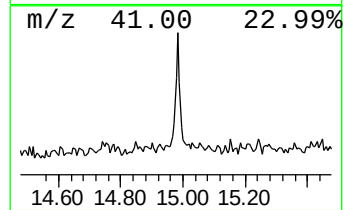
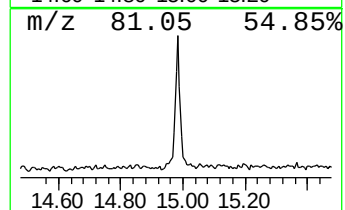
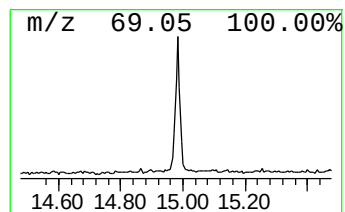
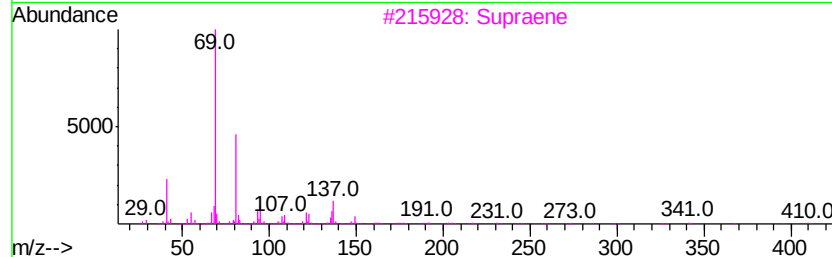
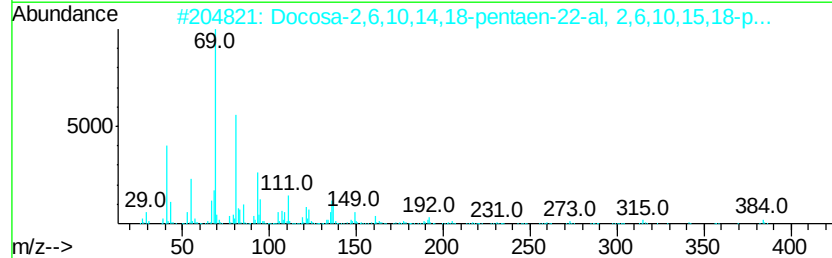
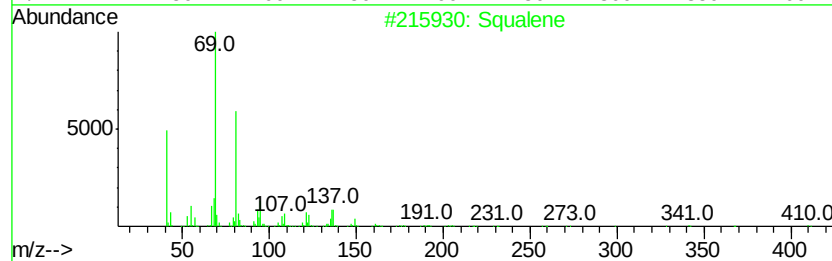
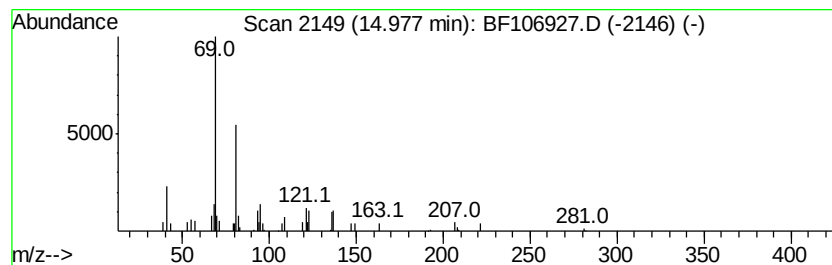
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Peak Number 4 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.16 ng	47909	Perylene-d12	15.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	000111-02-4 91
2	Docosa-2,6,10,14,18-pentaen-22-a...		384 C27H44O	1000163-04-7 86
3	Supraene		410 C30H50	007683-64-9 86
4	.beta.-d-Mannofuranoside, O-geranyl		316 C16H28O6	1000154-77-2 72
5	(.+/-)-Lavandulol, pentafluorop...		300 C13H17F5O2	1000352-63-1 72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	9.7	ng	197657	1	6.95	405708	20.0
unknown6.73	6.73	84.0	ng	1703740	1	6.95	405708	20.0
Squalene	14.98	2.2	ng	47909	6	15.68	443316	20.0