

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010517\
 Data File : BF092099.D
 Acq On : 5 Jan 2017 20:02
 Operator : UM/SJ
 Sample : I1004-10
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-19

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-BF122116.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	4.070	190	191	196	rBV	36743	69564	1.17%	0.162%
2	4.779	251	253	265	rVB	701691	825683	13.94%	1.925%
3	5.247	291	294	310	rVB	2641581	2651102	44.77%	6.181%
4	6.310	384	387	389	rBV	1585980	1773053	29.95%	4.134%
5	6.425	394	397	399	rBV	4812522	4809527	81.23%	11.214%
6	6.653	414	417	419	rBV	1106432	1149443	19.41%	2.680%
7	6.802	428	430	433	rBV	3019674	4085193	68.99%	9.525%
8	7.225	464	467	469	rBV	3830508	4010383	67.73%	9.350%
9	7.933	527	529	532	rBV	1236178	1436911	24.27%	3.350%
10	9.019	621	624	626	rBV	6107934	5921012	100.00%	13.805%
11	9.682	680	682	685	rBV	1627596	1625473	27.45%	3.790%
12	10.482	749	752	754	rBV	2815857	3965895	66.98%	9.247%
13	11.168	809	812	814	rBV	1531636	1680689	28.39%	3.919%
14	11.705	857	859	866	rBV2	69779	147727	2.49%	0.344%
15	12.494	926	928	935	rBV	119870	163432	2.76%	0.381%
16	12.757	948	951	953	rBV	5504459	5889457	99.47%	13.732%
17	13.797	1039	1042	1044	rBV	1251170	1487427	25.12%	3.468%
18	14.643	1113	1116	1118	rVB	151901	148854	2.51%	0.347%
19	15.168	1159	1162	1164	rBV	721575	1048832	17.71%	2.445%

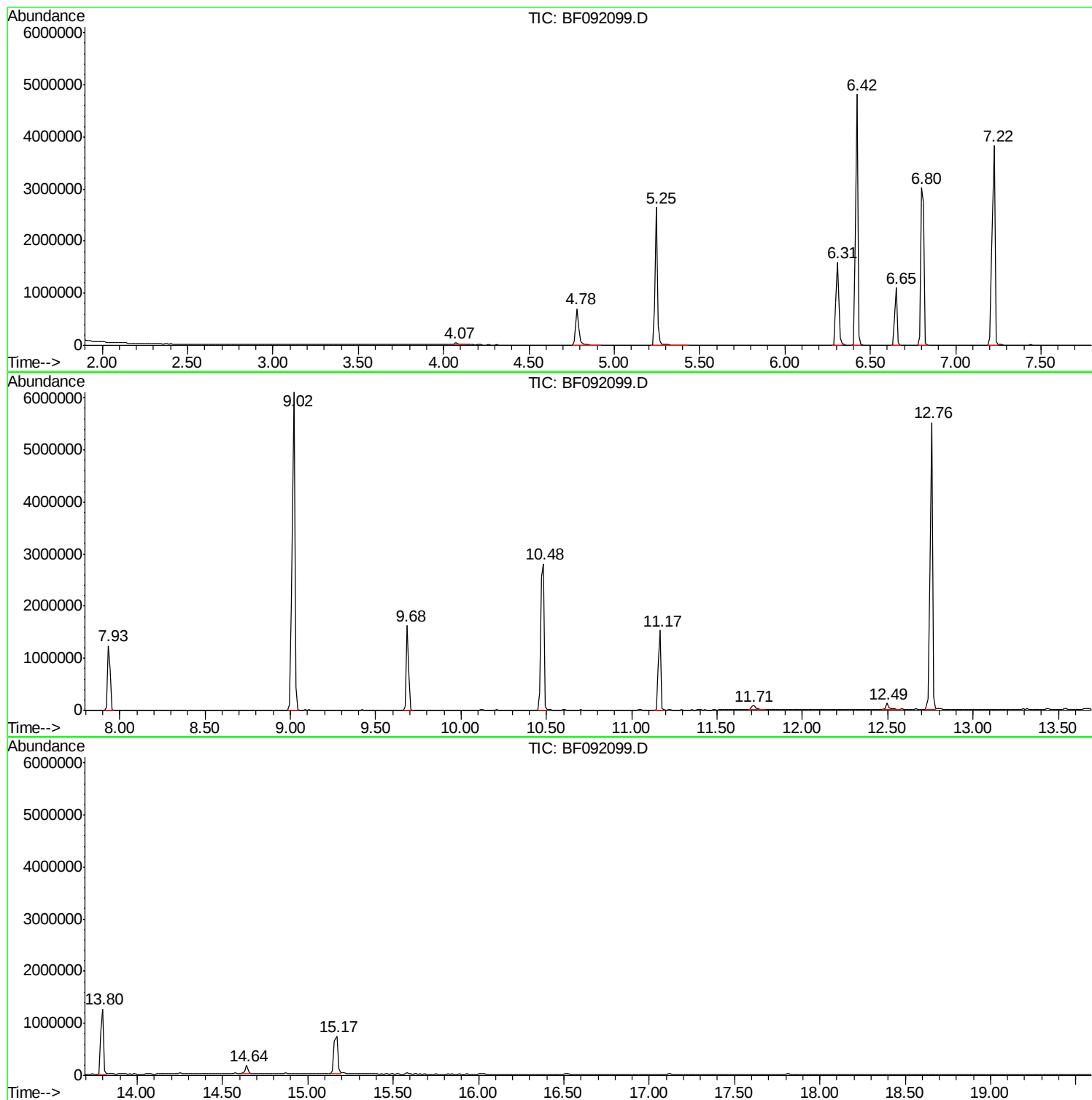
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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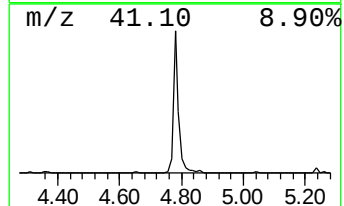
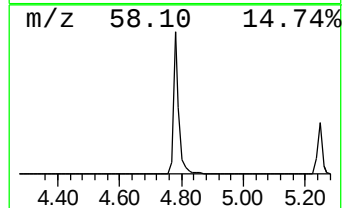
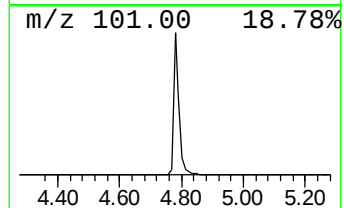
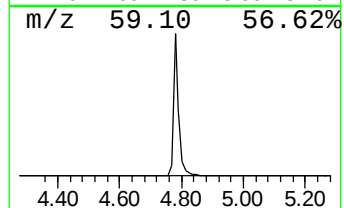
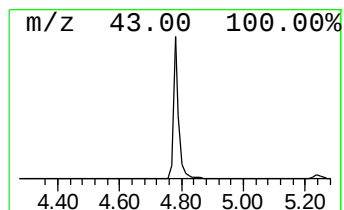
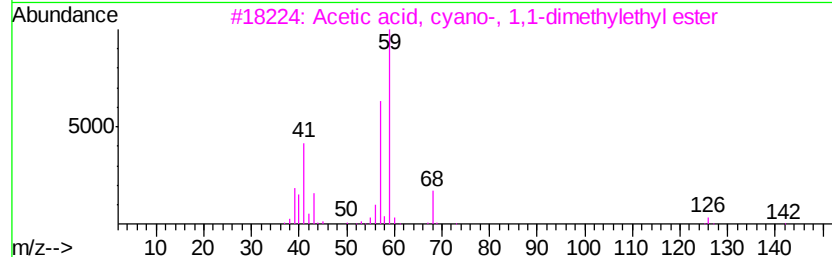
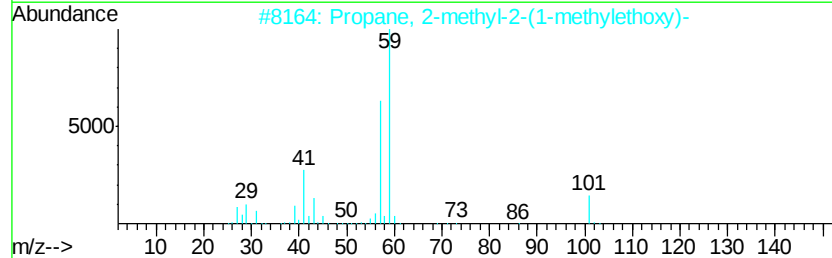
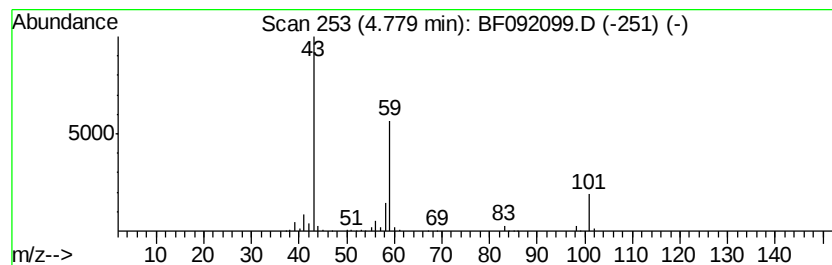
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	14.37 ng	825683	1,4-Dichlorobenzene-d4	6.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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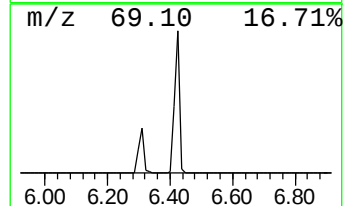
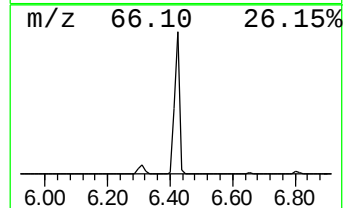
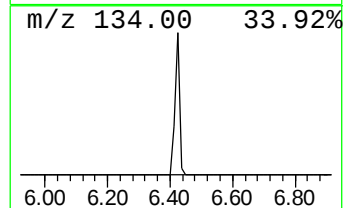
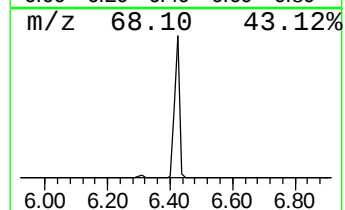
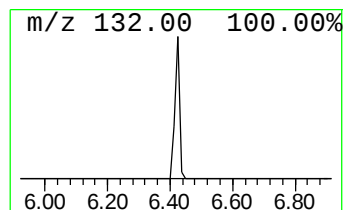
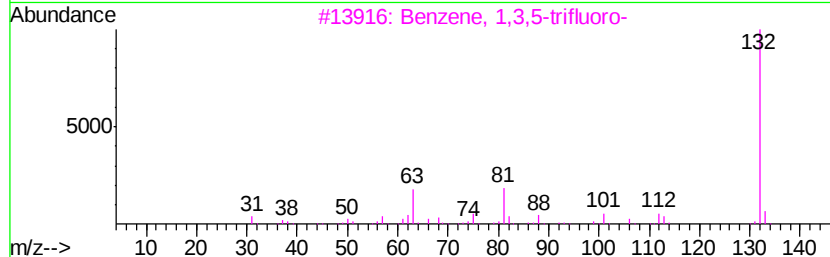
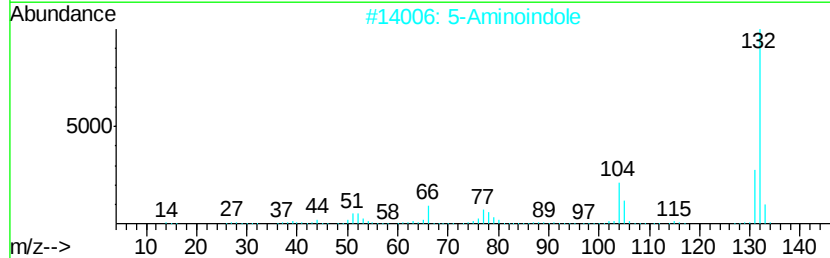
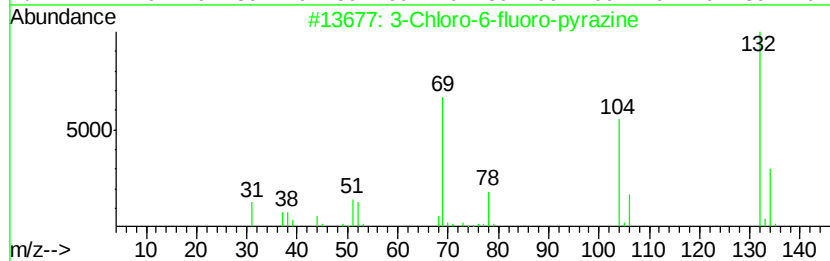
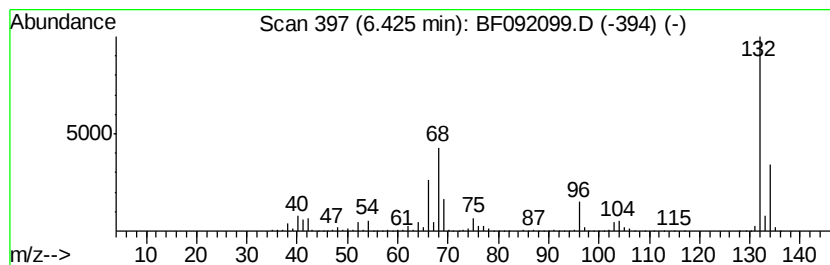
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Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	83.68 ng	4809530	1,4-Dichlorobenzene-d4	6.65

Hit#	of	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	12
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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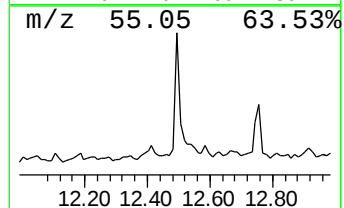
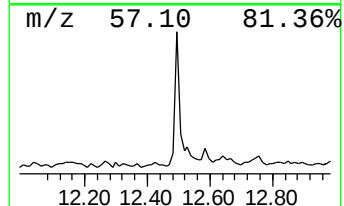
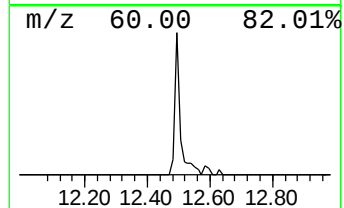
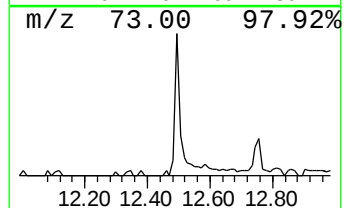
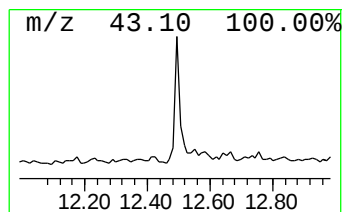
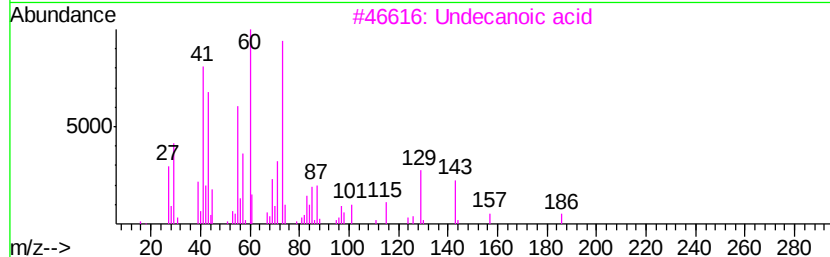
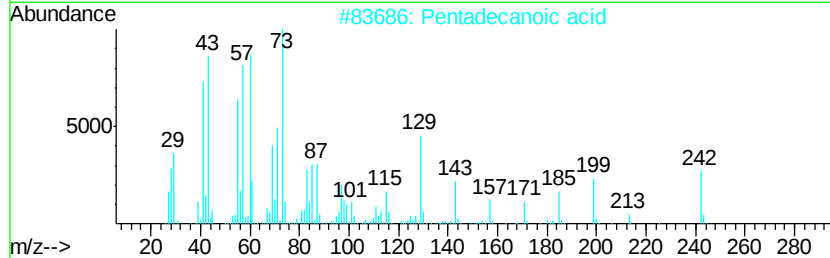
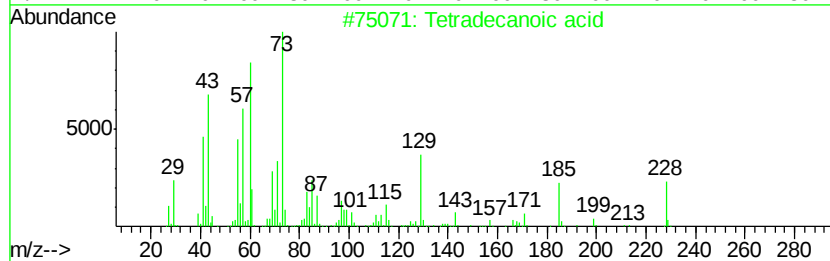
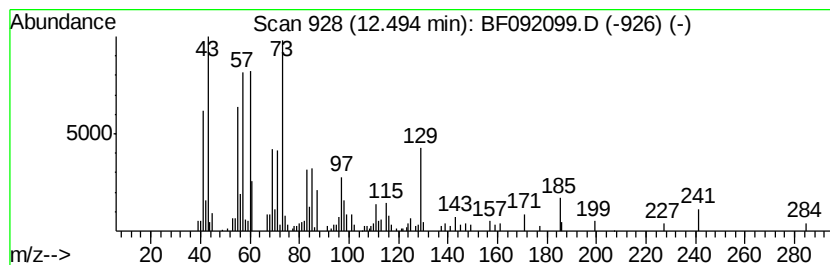
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Peak Number 4 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	2.20 ng	163432	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		Undecanoic acid	186	C11H22O2	000112-37-8	64
4		n-Decanoic acid	172	C10H20O2	000334-48-5	47
5		Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	27



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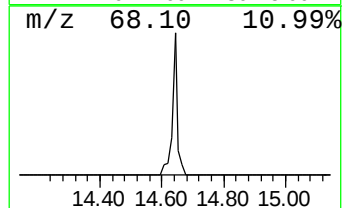
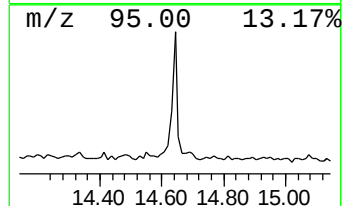
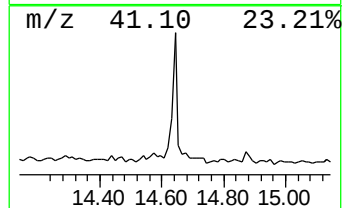
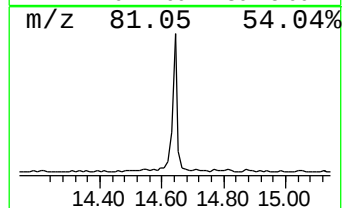
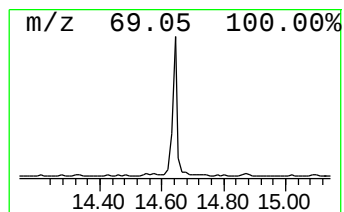
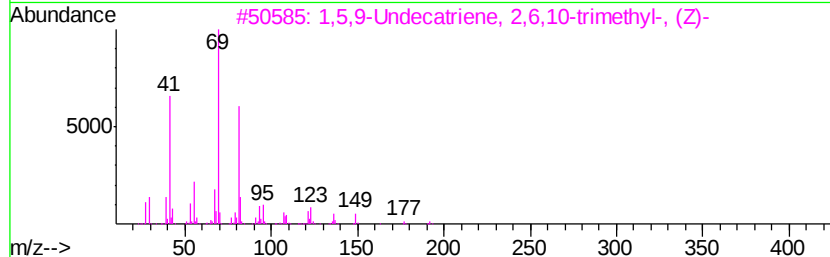
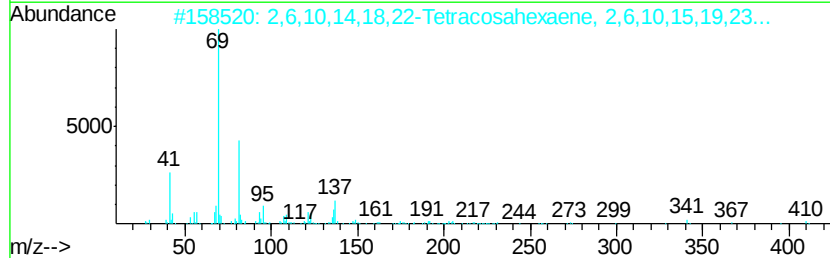
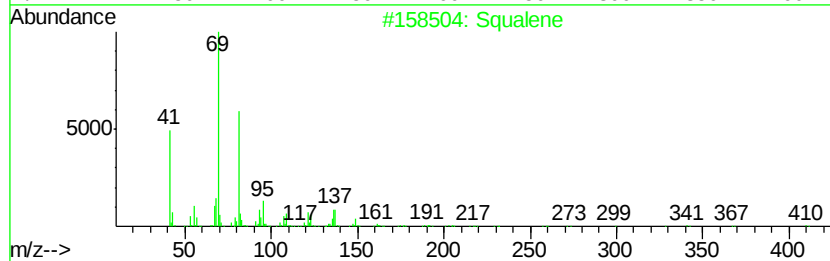
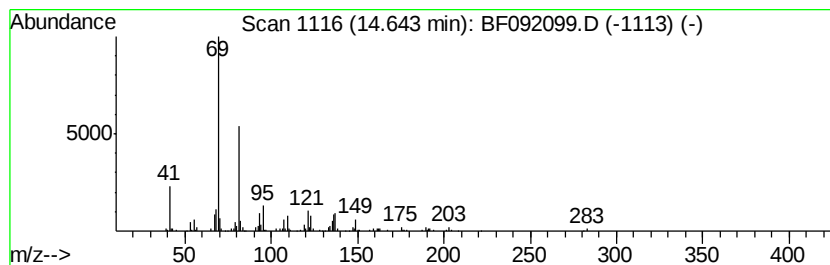
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.84 ng	148854	Perylene-d12	15.17
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	1,5,9-Undecatriene, 2,6,10-trime...		192 C14H24	062951-96-6 86
4	Propanoic acid, 2,2-dimethyl-, [...		306 C20H34O2	1000164-38-8 72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...		264 C17H28O2	004128-17-0 64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.78	14.4	ng	825683	1	6.65	1149440	20.0
unknown6.42	6.42	83.7	ng	4809530	1	6.65	1149440	20.0
Tetradecanoic acid	12.49	2.2	ng	163432	5	13.80	1487430	20.0
Squalene	14.64	2.8	ng	148854	6	15.17	1048830	20.0