

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
 Data File : BF092440.D
 Acq On : 24 Jan 2017 20:28
 Operator : UM/SJ
 Sample : I1322-02
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B2-8-9

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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	5.150	265	268	274	rVB	1039232	1564851	35.26%	4.137%
2	5.562	301	304	306	rBV	3732425	3777072	85.10%	9.986%
3	6.590	390	394	396	rBV	3284210	4438324	100.00%	11.734%
4	6.727	403	406	409	rBV	3257722	3679052	82.89%	9.727%
5	6.967	424	427	429	rBV	1114651	960713	21.65%	2.540%
6	7.127	438	441	443	rBV	2813387	3043958	68.58%	8.048%
7	7.527	473	476	479	rBV	2138600	2365779	53.30%	6.255%
8	8.259	537	540	542	rBV	1423303	1296227	29.21%	3.427%
9	9.345	632	635	637	rBV	4055979	4163596	93.81%	11.008%
10	9.733	667	669	671	rBV	186645	195282	4.40%	0.516%
11	10.019	692	694	697	rVB	988466	1392614	31.38%	3.682%
12	10.465	729	733	734	rBV2	76017	88710	2.00%	0.235%
13	10.819	761	764	766	rBV	2162729	2425384	54.65%	6.412%
14	10.934	772	774	779	rVB	92987	129298	2.91%	0.342%
15	11.391	812	814	815	rBV	79726	68722	1.55%	0.182%
16	11.516	823	825	827	rBV	1664329	1423950	32.08%	3.765%
17	12.042	869	871	873	rBV	75395	84504	1.90%	0.223%
18	13.105	962	964	967	rBV	2864703	4052154	91.30%	10.713%
19	13.997	1040	1042	1049	rBV	177879	263354	5.93%	0.696%
20	14.157	1053	1056	1058	rBV	1344178	1268107	28.57%	3.353%
21	15.025	1130	1132	1134	rBV	97265	102436	2.31%	0.271%
22	15.631	1182	1185	1188	rBV	706251	885098	19.94%	2.340%
23	15.688	1188	1190	1194	rVB	27517	48118	1.08%	0.127%
24	16.134	1226	1229	1231	rBV	31651	58234	1.31%	0.154%
25	16.648	1271	1274	1283	rVB2	22025	47950	1.08%	0.127%

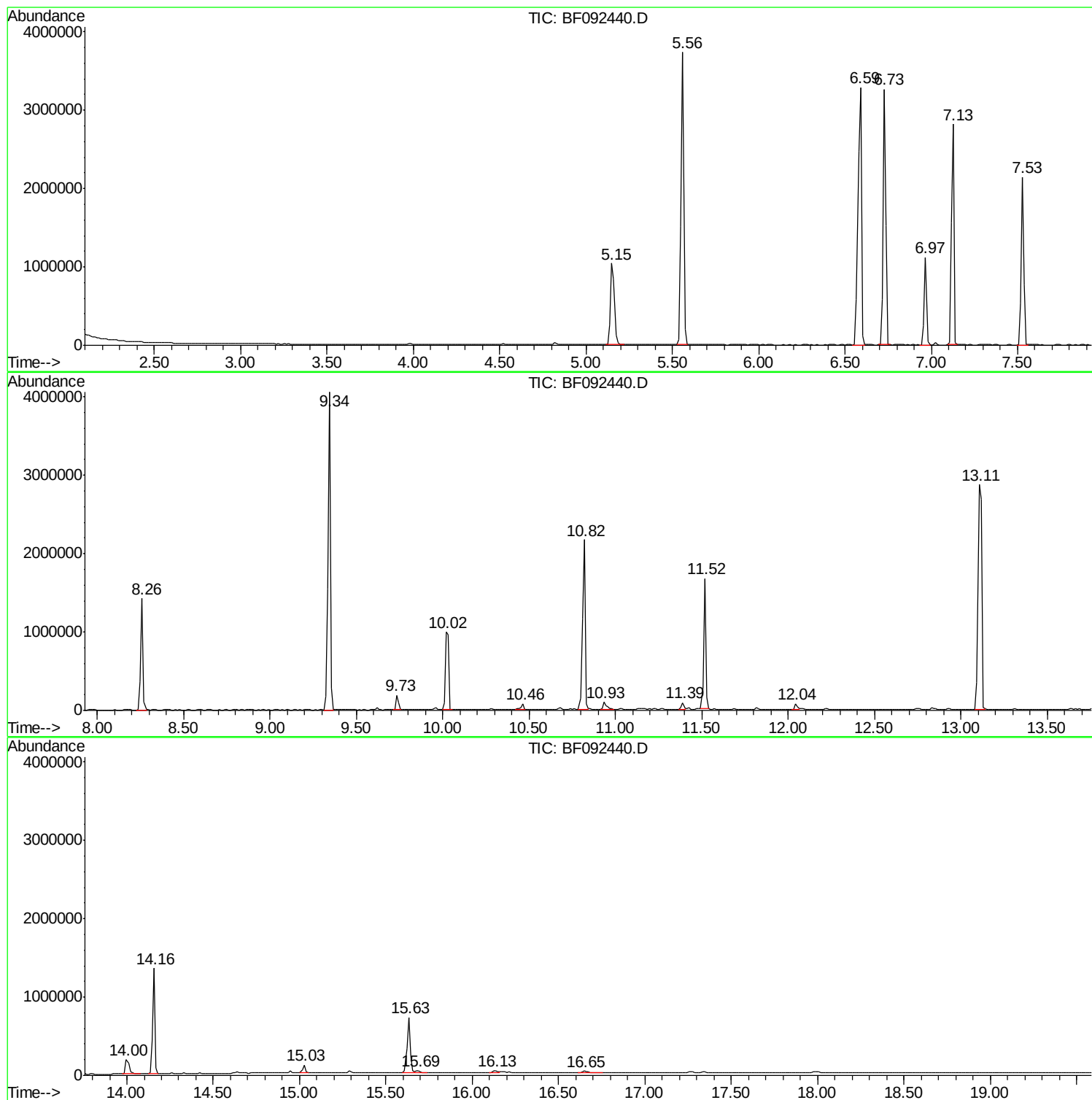
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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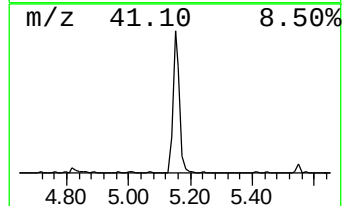
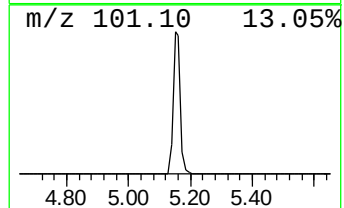
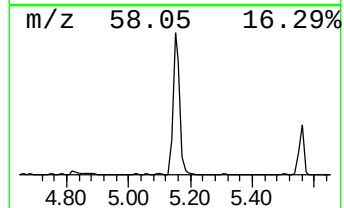
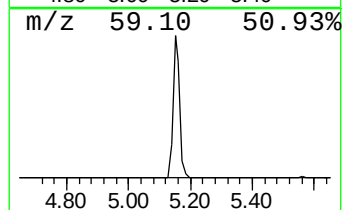
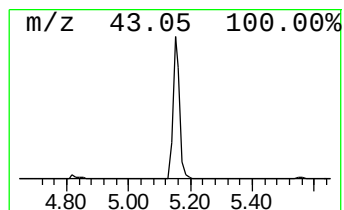
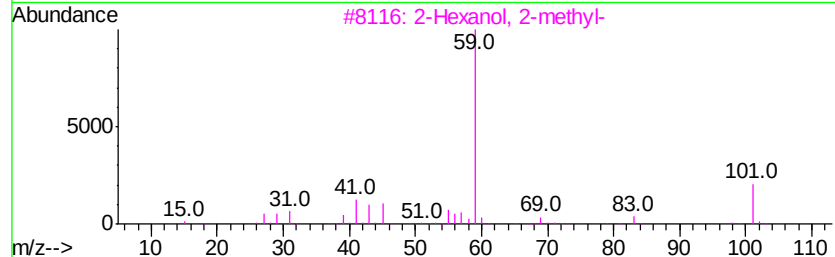
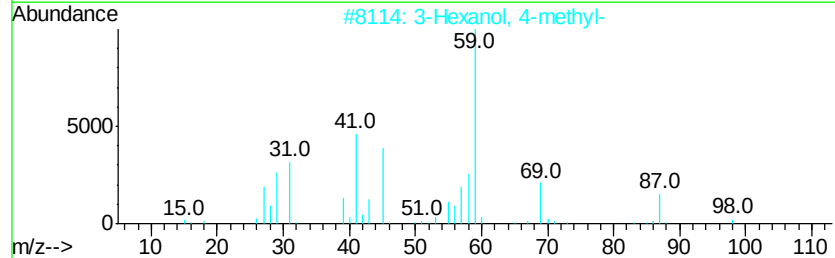
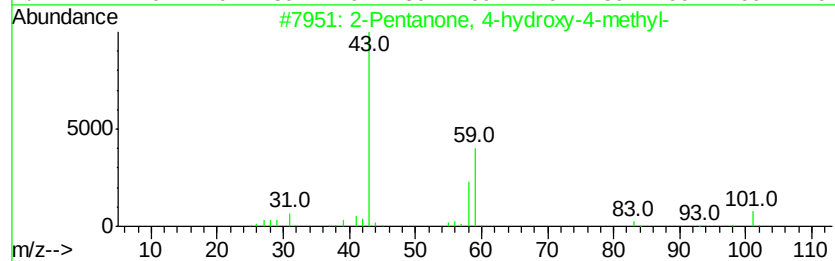
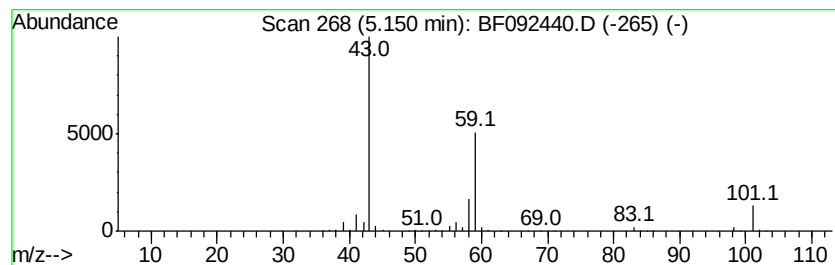
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
5.15	32.58 ng	1564850	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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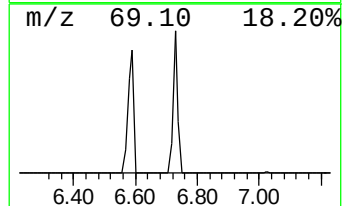
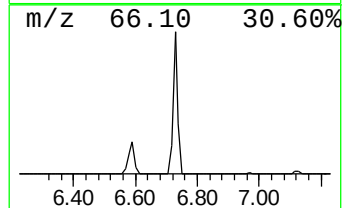
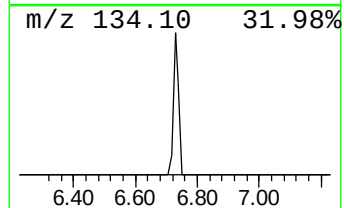
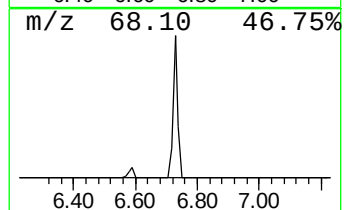
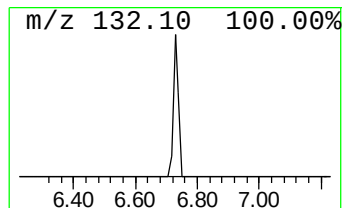
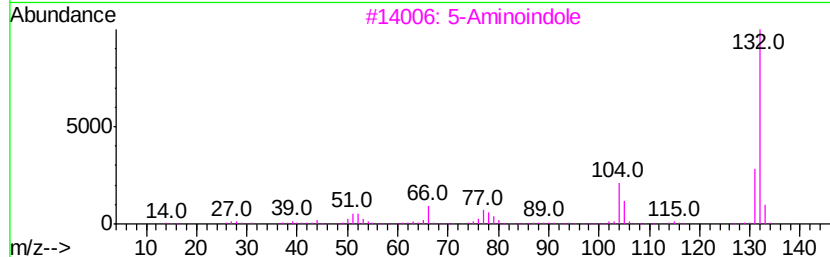
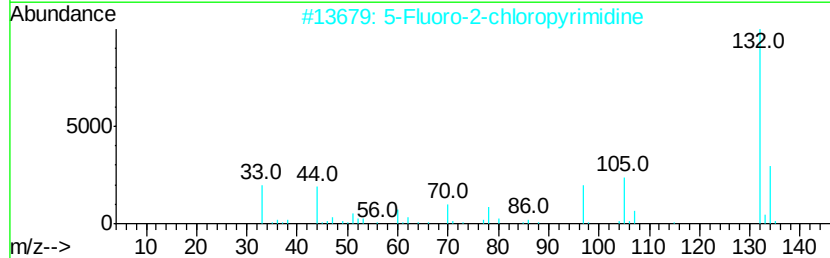
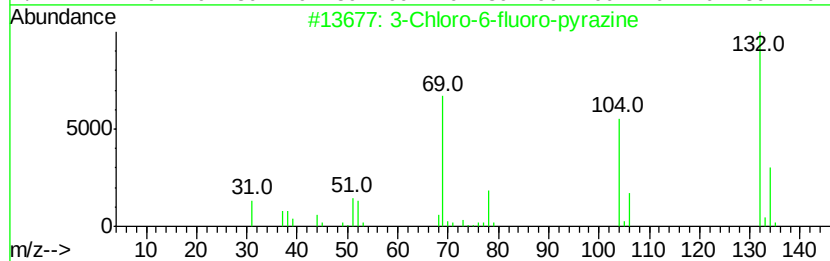
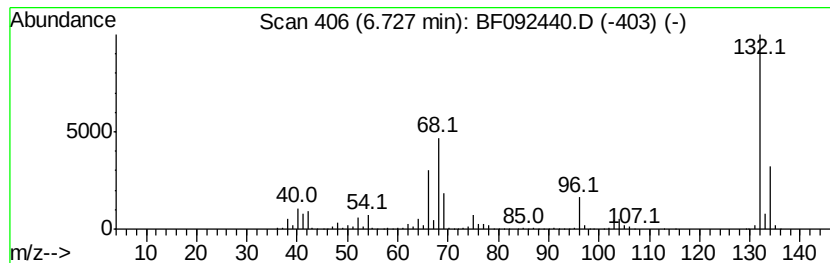
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Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	76.59 ng	3679050	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



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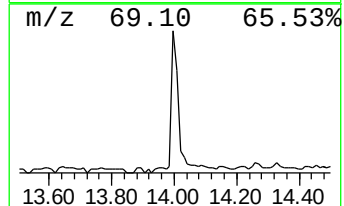
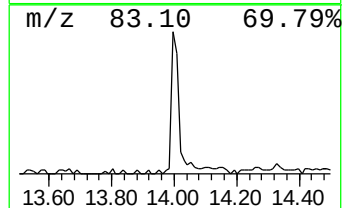
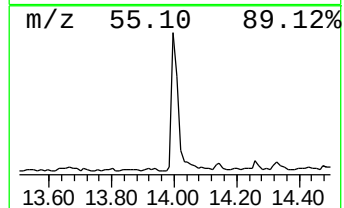
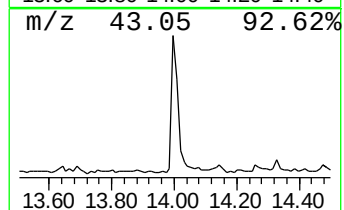
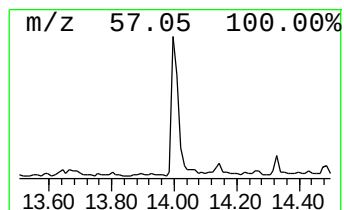
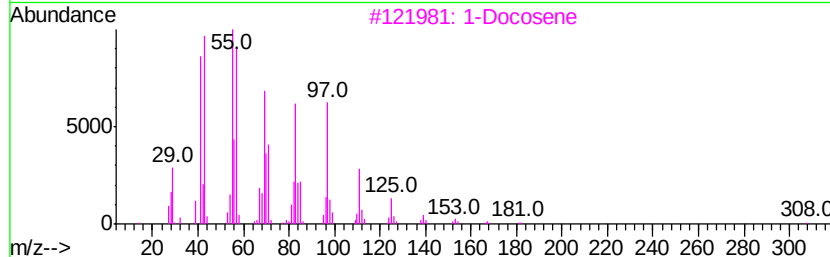
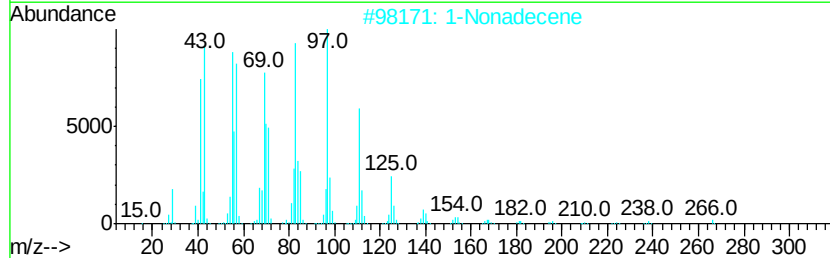
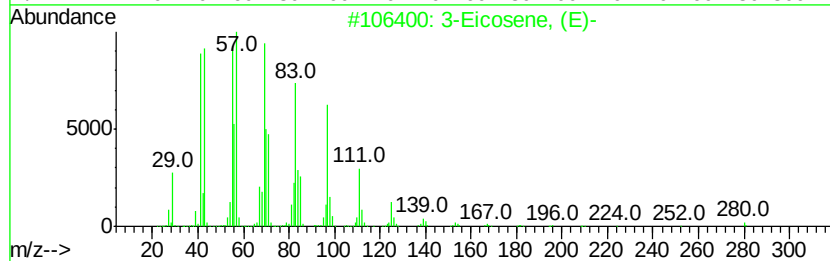
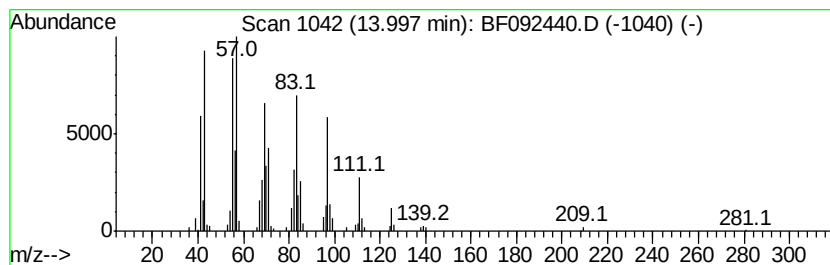
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Peak Number 4 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.00	4.15 ng	263354	Chrysene-d12	14.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



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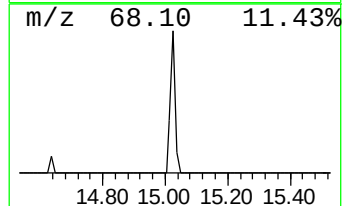
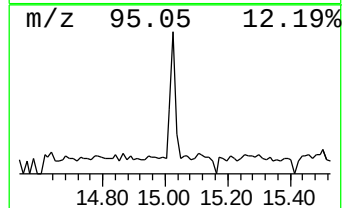
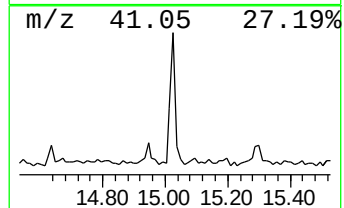
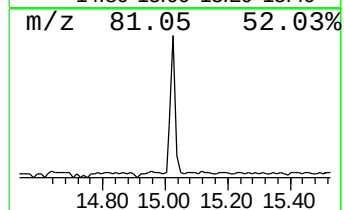
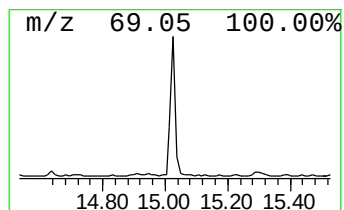
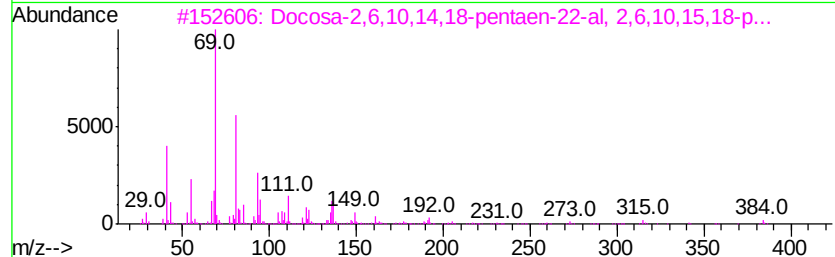
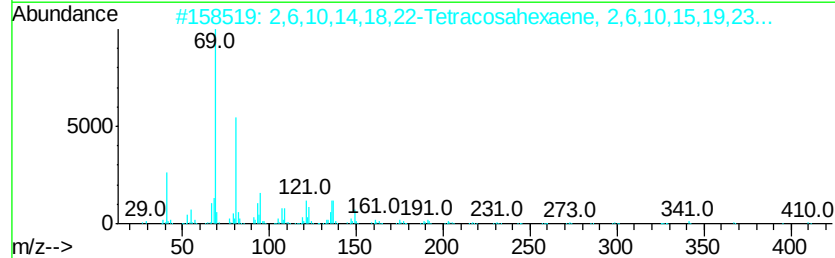
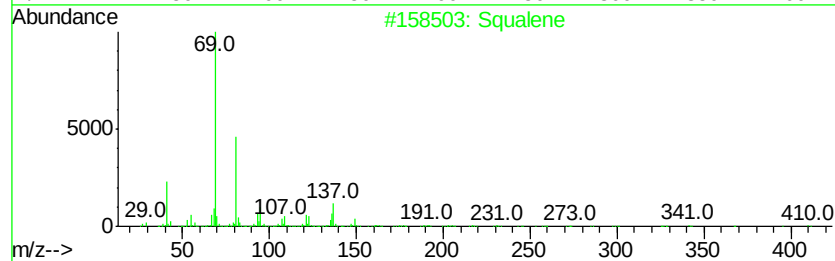
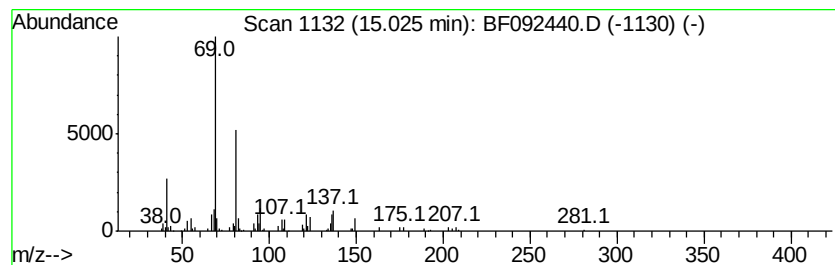
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	2.31 ng	102436	Perylene-d12	15.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	32.6	ng	1564850	1	6.97	960713	20.0
unknown6.73	6.73	76.6	ng	3679050	1	6.97	960713	20.0
3-Eicosene, (E)-	14.00	4.2	ng	263354	5	14.16	1268110	20.0
Squalene	15.03	2.3	ng	102436	6	15.63	885098	20.0