

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091018\
 Data File : BF108899.D
 Acq On : 10 Sep 2018 18:03
 Operator : JU/SJ
 Sample : J4836-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-GF-02-025-B

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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	4.943	439	443	452	rVB	132504	161119	4.04%	0.455%
2	5.354	508	513	516	rBV	3931003	3739239	93.74%	10.555%
3	6.378	682	687	690	rBV	4022002	3896374	97.68%	10.998%
4	6.513	705	710	713	rBV	4095274	3872211	97.08%	10.930%
5	6.572	717	720	727	rVB	65717	59673	1.50%	0.168%
6	6.742	745	749	752	rBV	1515431	1189863	29.83%	3.359%
7	6.901	771	776	779	rBV	3280774	3025345	75.85%	8.540%
8	7.301	839	844	847	rBV	2655624	2391850	59.96%	6.751%
9	8.019	963	966	970	rBV	1587163	1437271	36.03%	4.057%
10	9.095	1145	1149	1153	rBV	4361721	3988821	100.00%	11.259%
11	9.219	1167	1170	1174	rVB	236667	208233	5.22%	0.588%
12	9.489	1212	1216	1219	rBV	962471	745409	18.69%	2.104%
13	9.772	1260	1264	1268	rBV	1761099	1399477	35.08%	3.950%
14	10.360	1359	1364	1370	rBV	39379	42564	1.07%	0.120%
15	10.554	1393	1397	1413	rBV	2220279	2028553	50.86%	5.726%
16	11.248	1511	1515	1519	rBV	1479411	1218244	30.54%	3.439%
17	11.783	1603	1606	1616	rBV3	71890	106106	2.66%	0.300%
18	12.830	1780	1784	1788	rBV	3435791	3249078	81.45%	9.171%
19	13.742	1935	1939	1943	rBV2	167064	259772	6.51%	0.733%
20	13.877	1958	1962	1965	rBV	1488633	1321297	33.13%	3.730%
21	14.660	2093	2095	2104	rVB	170014	224723	5.63%	0.634%
22	15.289	2198	2202	2206	rVB	761321	861896	21.61%	2.433%

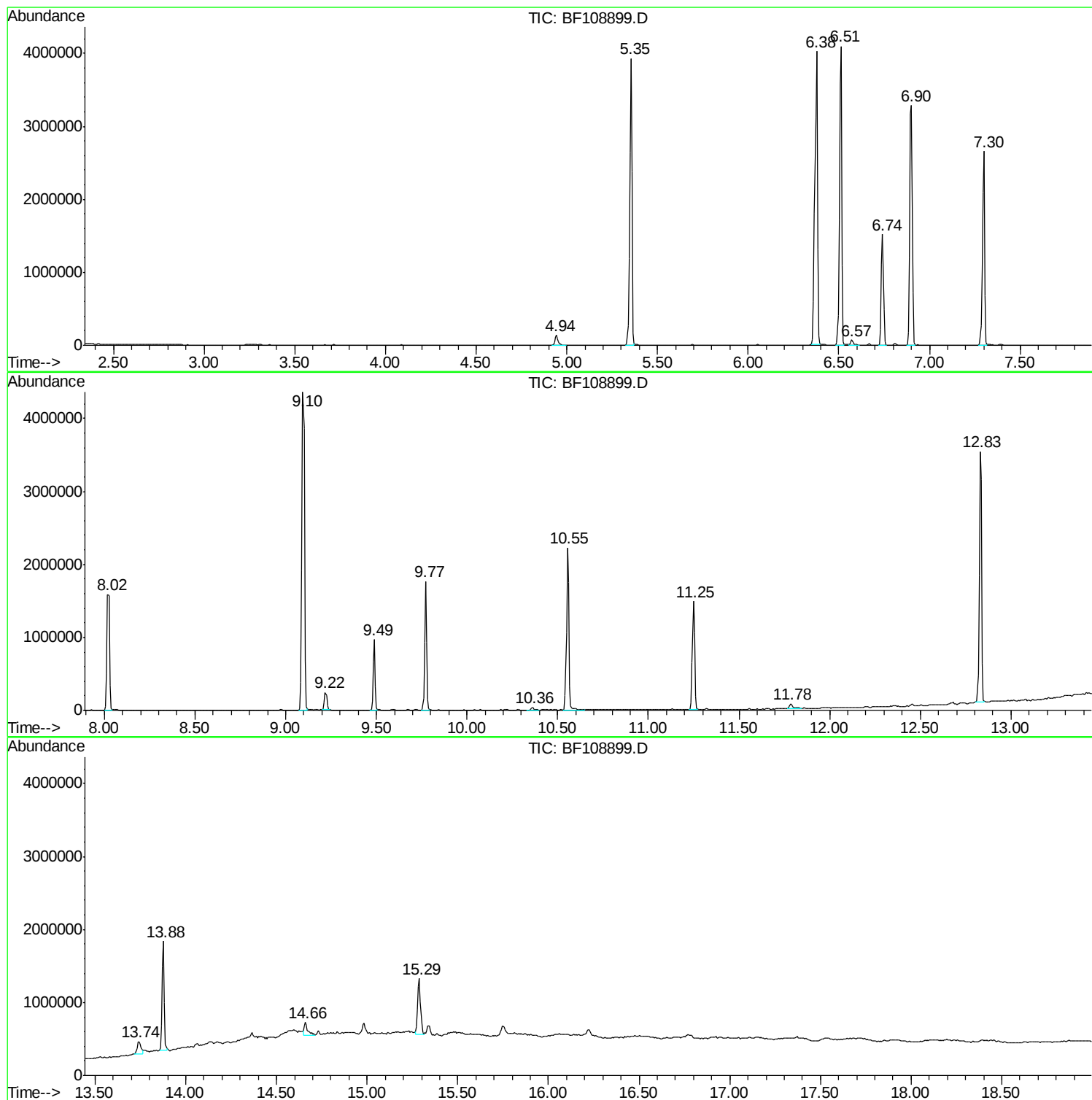
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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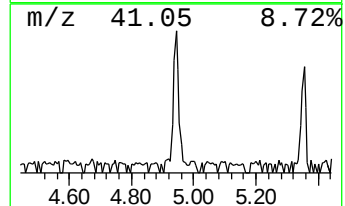
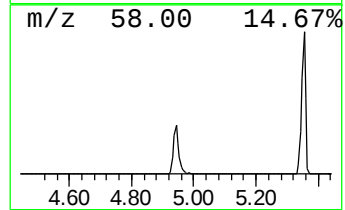
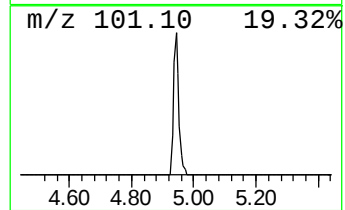
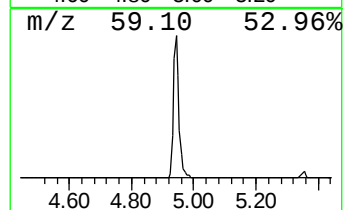
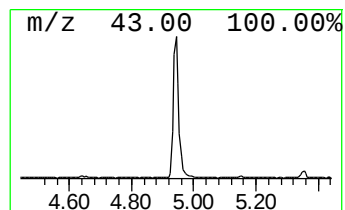
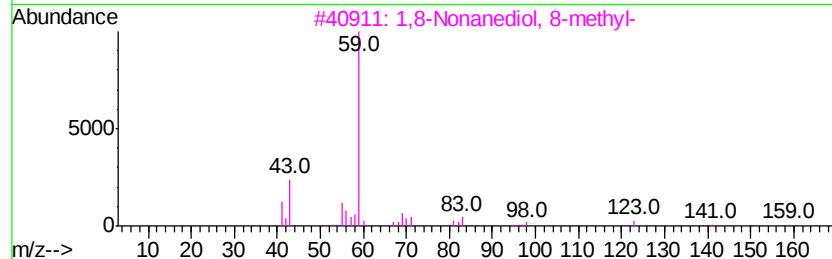
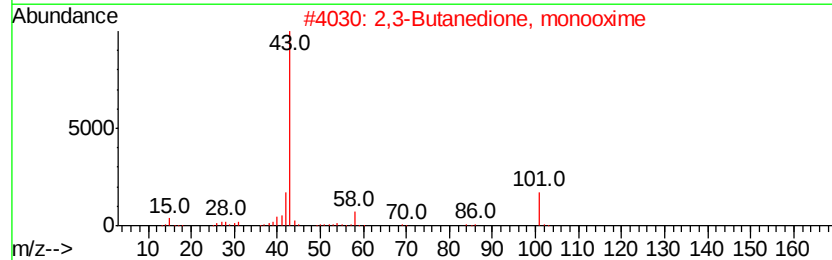
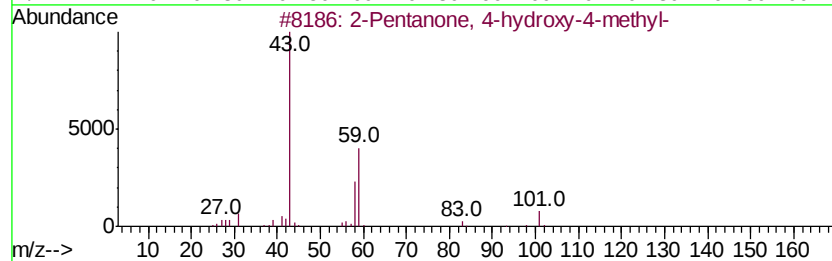
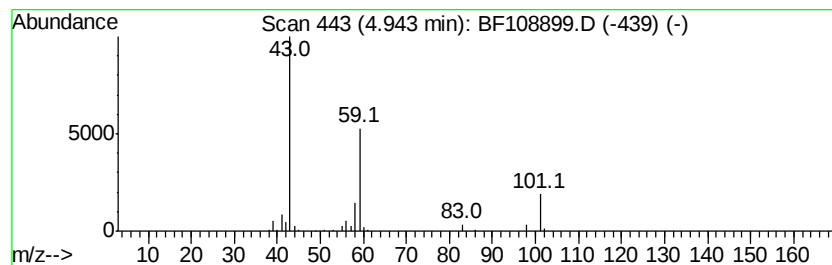
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	2.71 ng	161119	1,4-Dichlorobenzene-d4	6.74

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			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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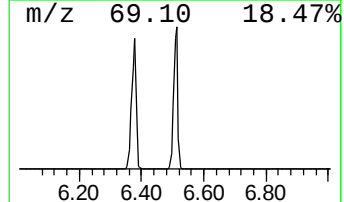
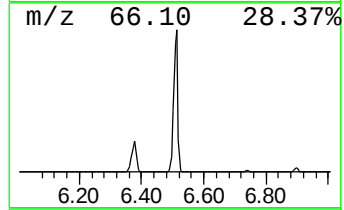
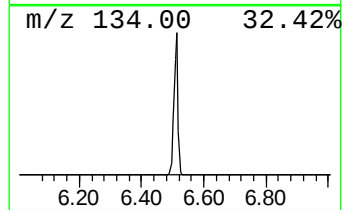
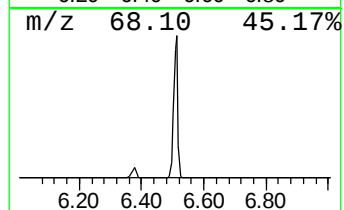
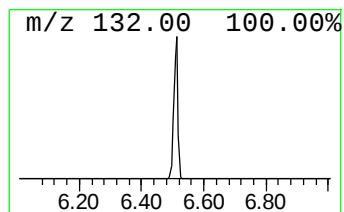
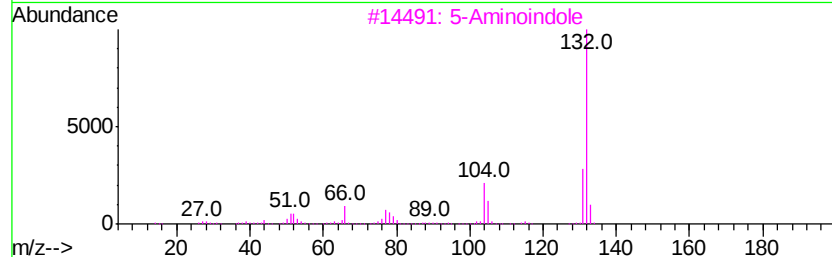
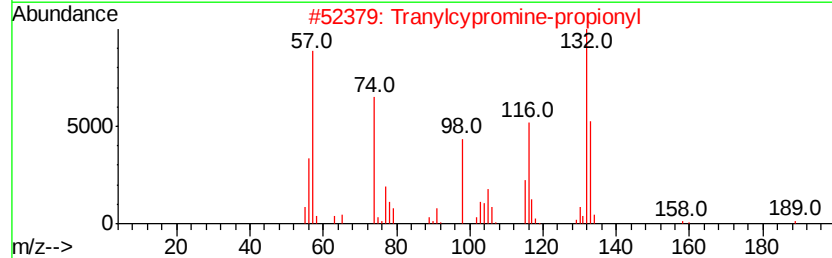
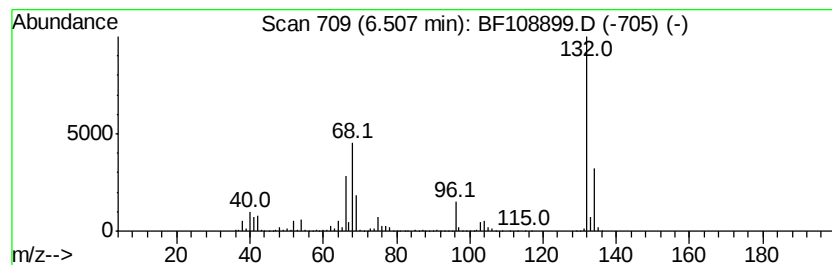
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	65.09 ng	3872210	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10	
3	5-Aminoindole	132	C8H8N2	005192-03-0	9	
4	Xenon	132	Xe	007440-63-3	9	
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9	



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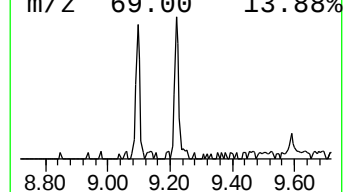
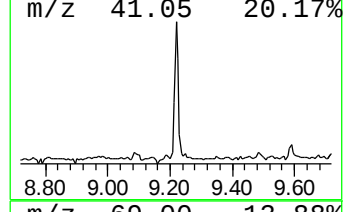
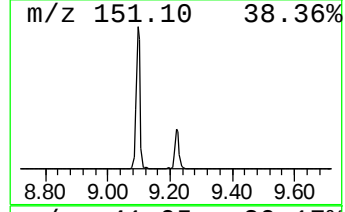
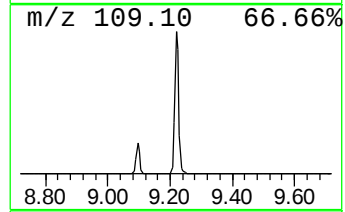
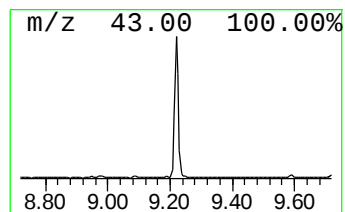
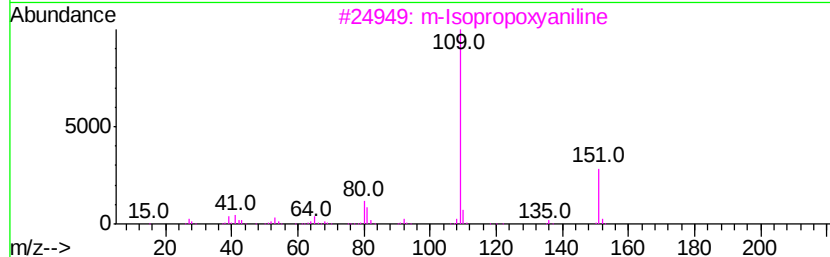
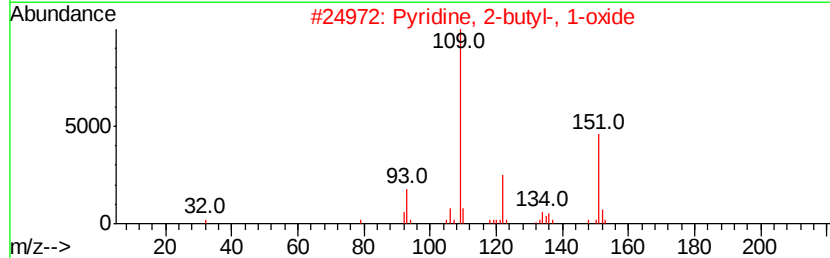
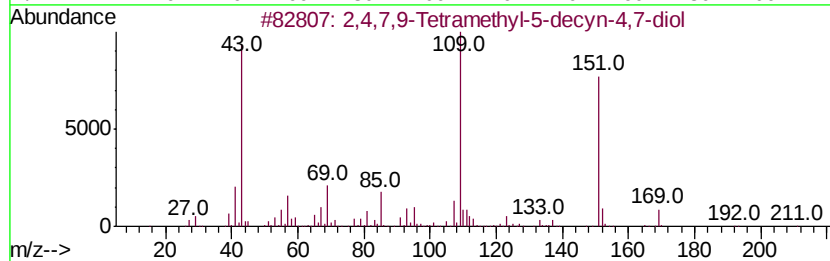
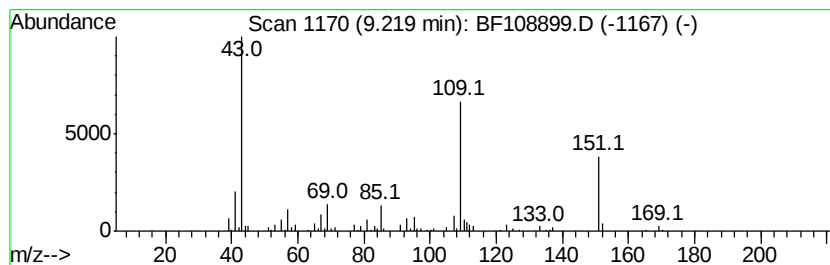
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Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.22	2.98 ng	208233	Acenaphthene-d10	9.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	59
3	m-Isopropoxvaniline	151	C9H13NO		041406-00-2	53
4	p-Isopropoxvaniline	151	C9H13NO		007664-66-6	53
5	Metacetamol	151	C8H9NO2		000621-42-1	53



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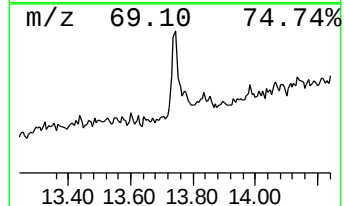
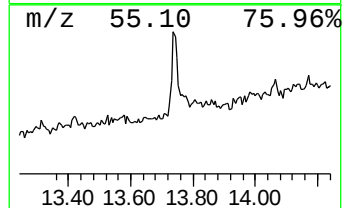
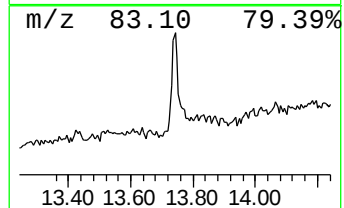
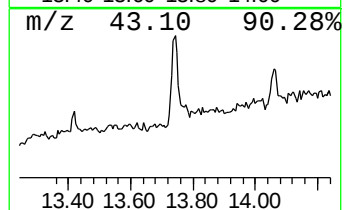
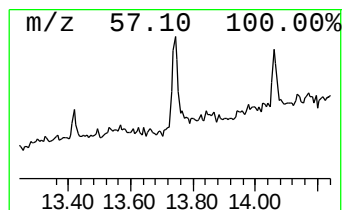
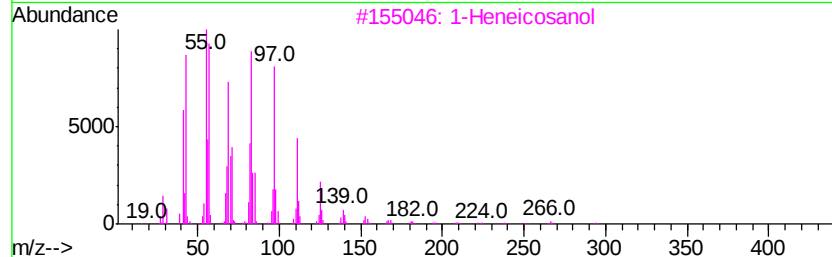
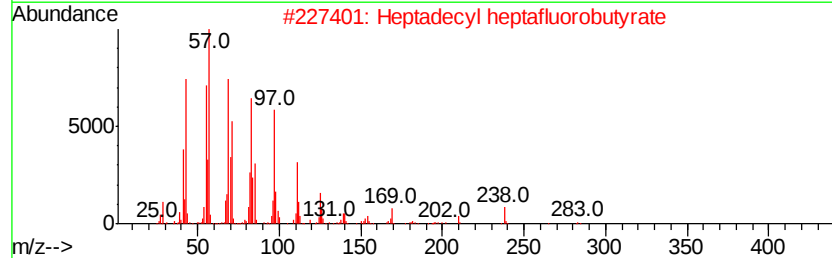
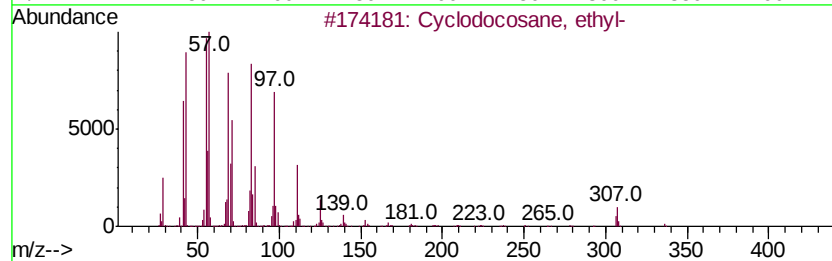
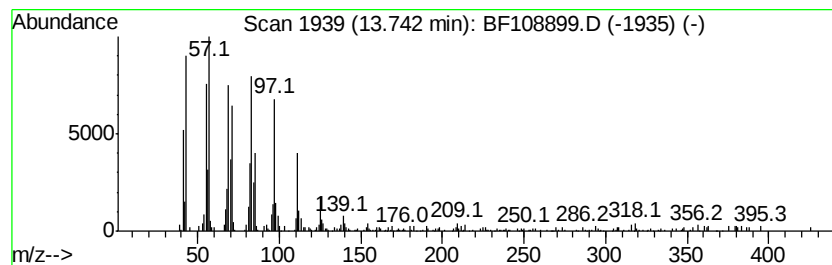
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Peak Number 5 Cyclodocosane, ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	3.93 ng	259772	Chrysene-d12	13.88	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	96
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	90



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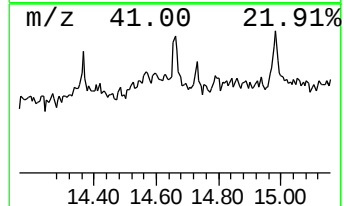
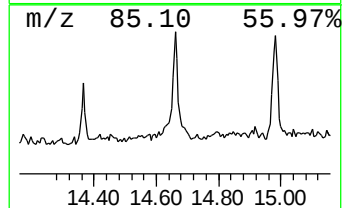
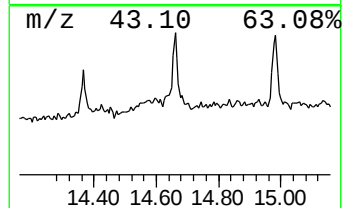
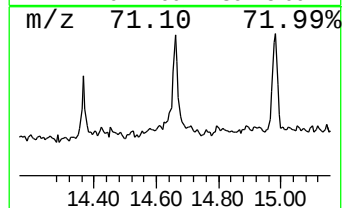
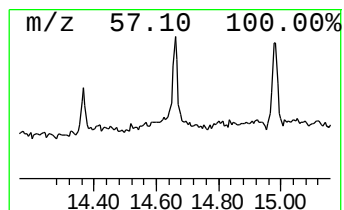
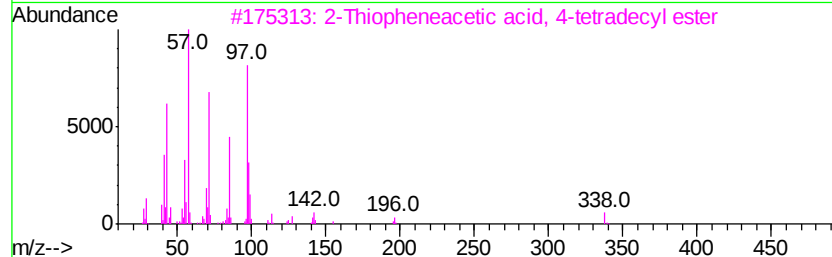
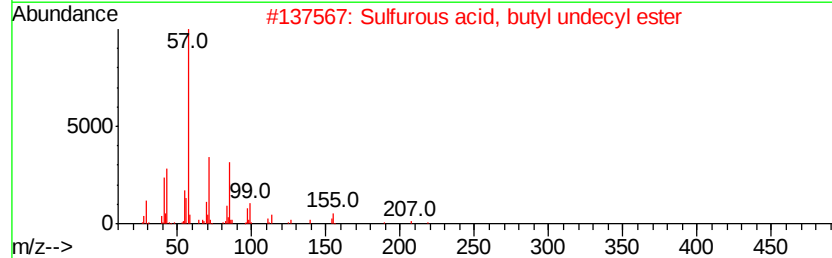
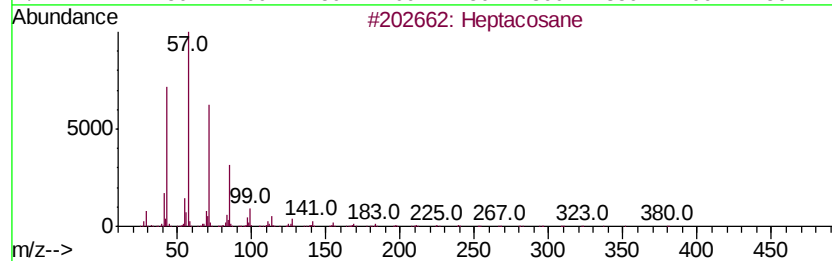
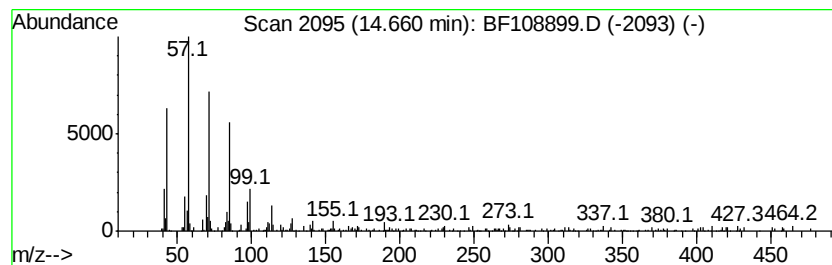
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Peak Number 6 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	5.21 ng	224723	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	93
2	Sulfurous acid, butyl undecyl ester		292	C15H32O3S	1000309-17-8	80
3	2-Thiopheneacetic acid, 4-tetrad...		338	C20H34O2S	1000280-67-0	80
4	Tetracosane		338	C24H50	000646-31-1	80
5	Heptadecane, 3-methyl-		254	C18H38	006418-44-6	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.94	2.7	ng	161119	1	6.74	1189860	20.0
unknown6.51	6.51	65.1	ng	3872210	1	6.74	1189860	20.0
2,4,7,9-Tetrameth...	9.22	3.0	ng	208233	3	9.77	1399480	20.0
Cyclodocosane, et...	13.74	3.9	ng	259772	5	13.88	1321300	20.0
Heptacosane	14.66	5.2	ng	224723	6	15.29	861896	20.0