

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092916\
 Data File : BF090301.D
 Acq On : 29 Sep 2016 20:38
 Operator : UM/SJ
 Sample : H4998-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B044-6-9

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-BF092016.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	1.644	3	5	41	rVB	1138080	2940315	100.00%	11.872%
2	4.536	255	258	268	rBV	351629	553155	18.81%	2.233%
3	5.016	298	300	303	rBV	1625819	2226474	75.72%	8.990%
4	6.124	394	397	399	rBV	2129389	2347550	79.84%	9.479%
5	6.227	404	406	409	rVV	2339799	2299025	78.19%	9.283%
6	6.456	424	426	429	rBV	525328	652534	22.19%	2.635%
7	6.616	437	440	443	rBV	1979703	1809945	61.56%	7.308%
8	7.039	474	477	479	rBV	1338507	1560851	53.08%	6.302%
9	7.176	487	489	495	rVB	30554	37250	1.27%	0.150%
10	7.747	537	539	542	rBV	833621	833679	28.35%	3.366%
11	8.833	631	634	637	rBV	2669801	2389144	81.25%	9.647%
12	9.233	667	669	672	rBV	935652	1094400	37.22%	4.419%
13	9.496	690	692	694	rBV	1115175	920824	31.32%	3.718%
14	9.930	724	730	731	rBV	18416	38317	1.30%	0.155%
15	9.953	731	732	734	rVB	25153	35127	1.19%	0.142%
16	10.182	748	752	753	rBV	28050	44819	1.52%	0.181%
17	10.285	758	761	763	rBV	1245161	1278003	43.46%	5.160%
18	10.433	771	774	777	rVB	49445	84189	2.86%	0.340%
19	10.868	811	812	814	rBV	21291	30254	1.03%	0.122%
20	10.970	818	821	823	rBV	634113	698928	23.77%	2.822%
21	11.222	841	843	847	rVB	60274	77974	2.65%	0.315%
22	12.548	957	959	962	rBV	1244899	1525342	51.88%	6.159%
23	13.474	1037	1040	1047	rBV	90430	151910	5.17%	0.613%
24	13.576	1047	1049	1052	rBV	482974	632168	21.50%	2.553%
25	14.102	1093	1095	1099	rBV	22809	36334	1.24%	0.147%
26	14.902	1163	1165	1168	rBV	359881	467858	15.91%	1.889%

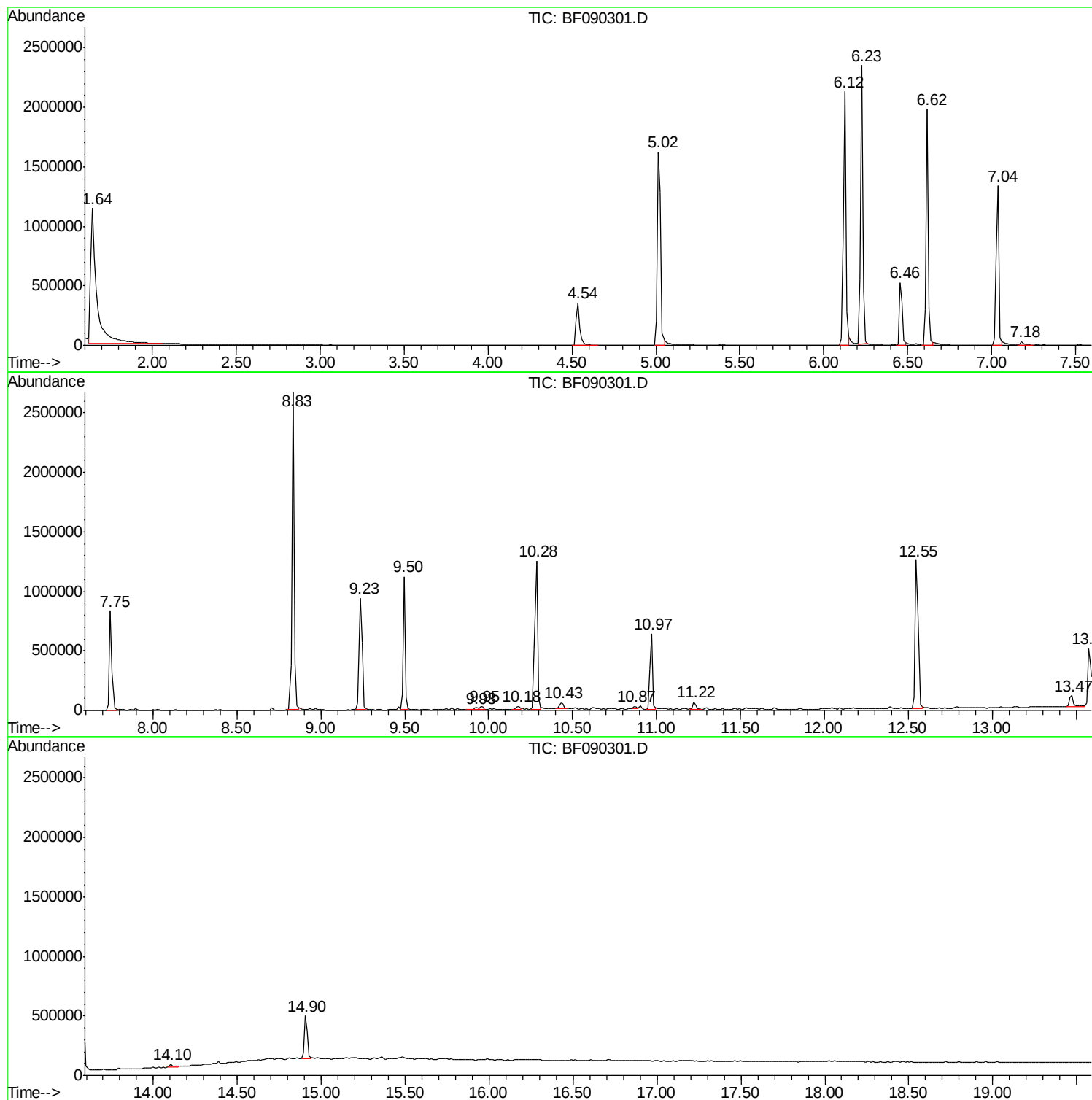
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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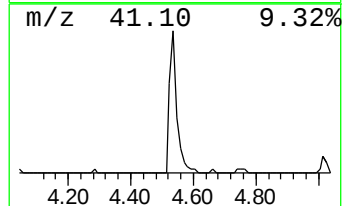
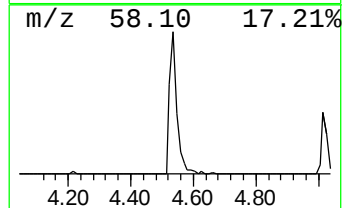
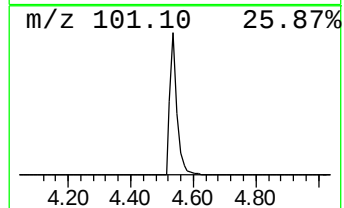
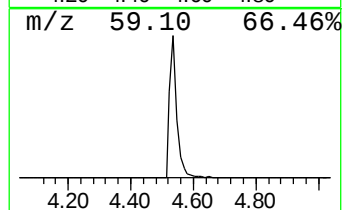
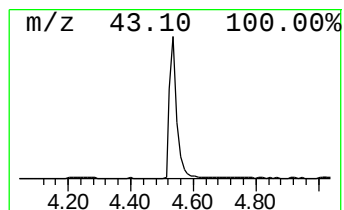
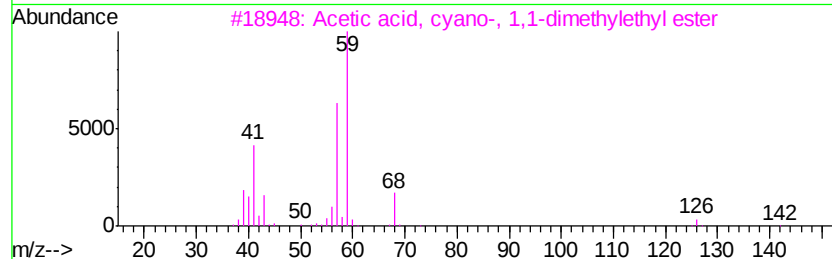
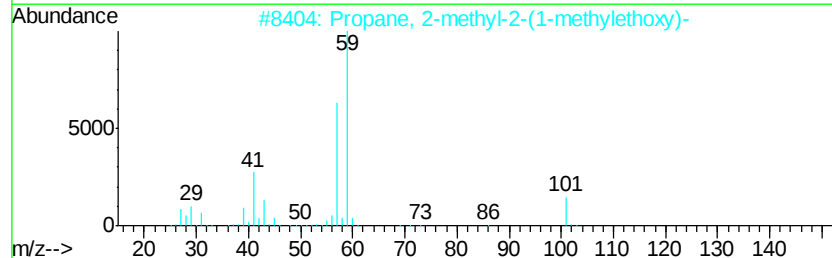
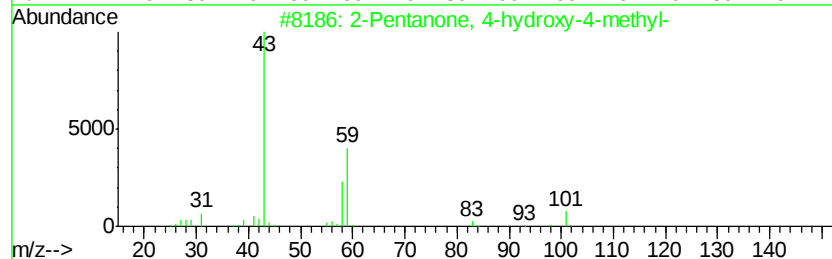
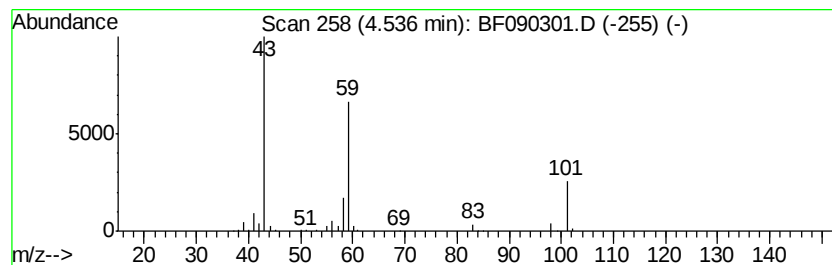
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	16.95 ng	553155	1,4-Dichlorobenzene-d4	6.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	50
3		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
4		Acetone	58	C3H6O	000067-64-1	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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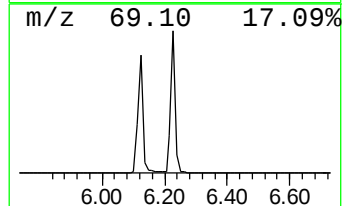
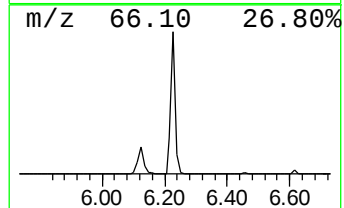
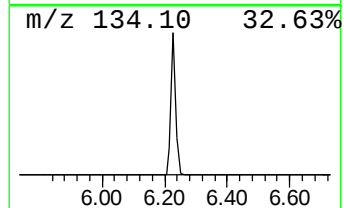
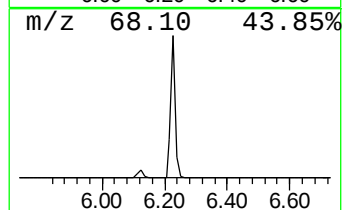
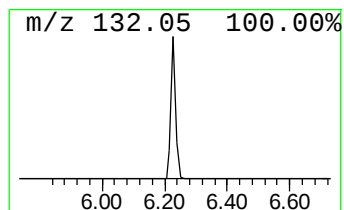
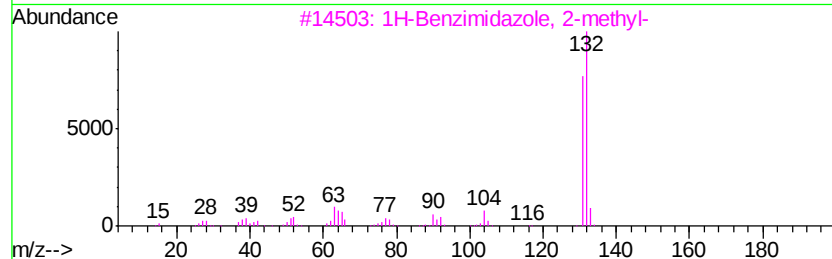
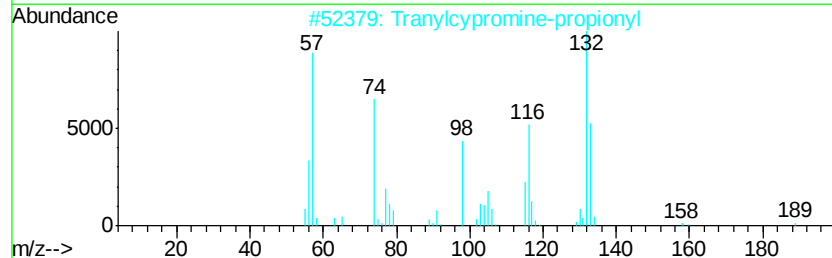
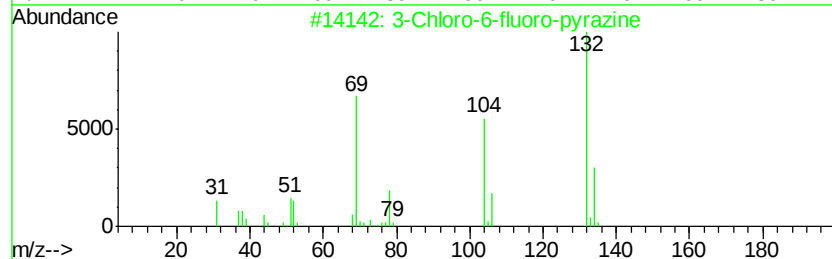
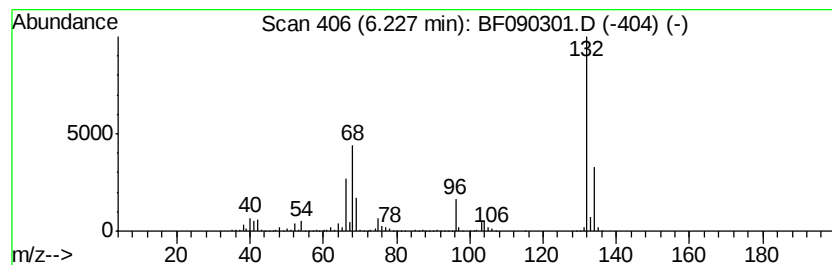
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Peak Number 3 unknown6.23 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.23	70.46 ng	2299030	1,4-Dichlorobenzene-d4	6.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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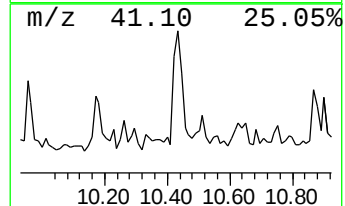
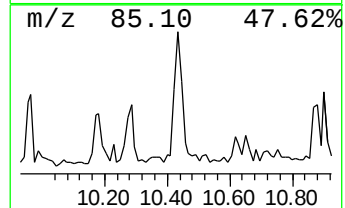
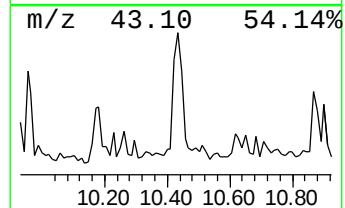
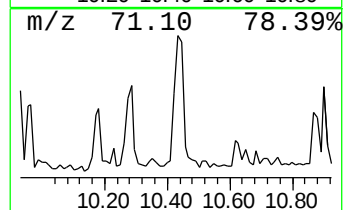
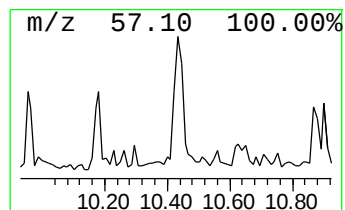
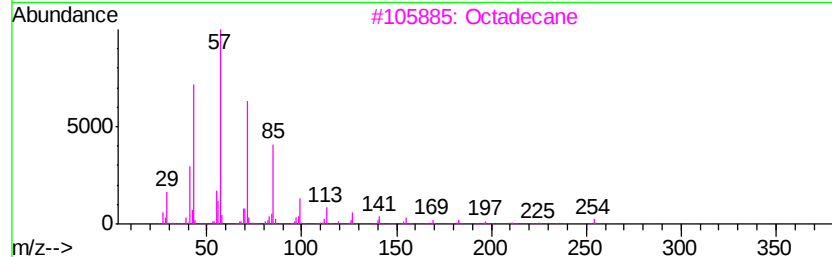
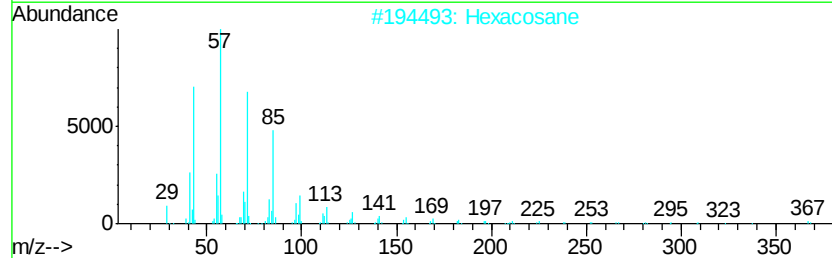
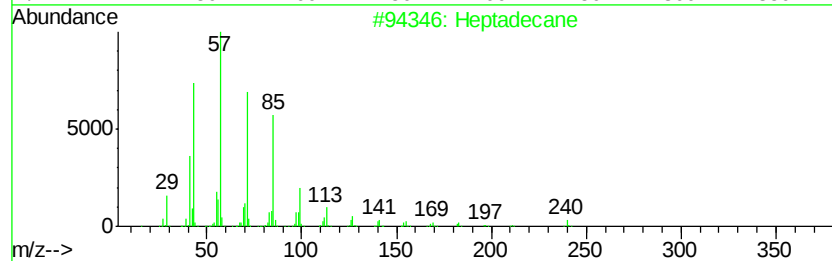
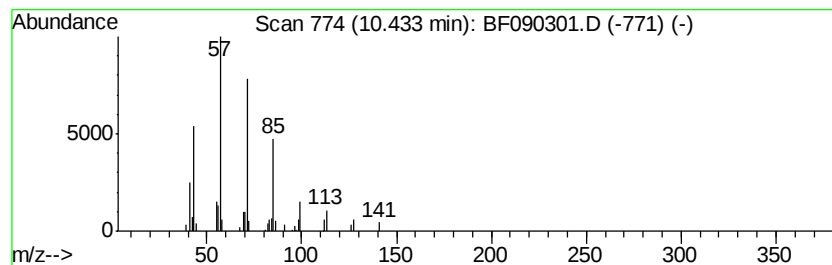
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Peak Number 5 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.41 ng	84189	Phenanthrene-d10	10.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Hexacosane		366	C26H54	000630-01-3	90
3	Octadecane		254	C18H38	000593-45-3	90
4	Hexadecane		226	C16H34	000544-76-3	90
5	Tetratetracontane		619	C44H90	007098-22-8	83



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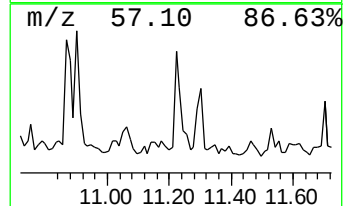
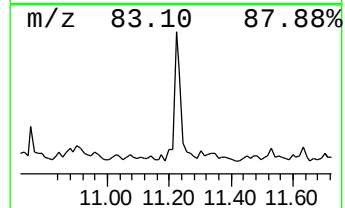
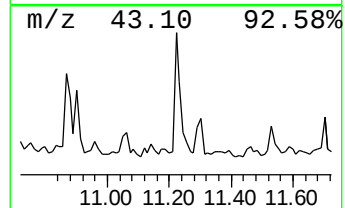
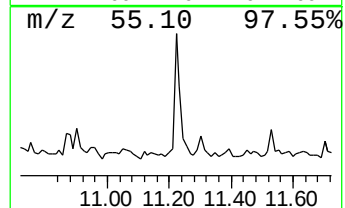
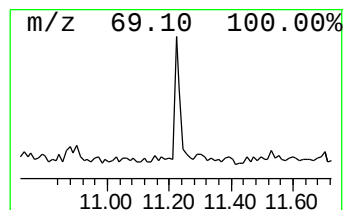
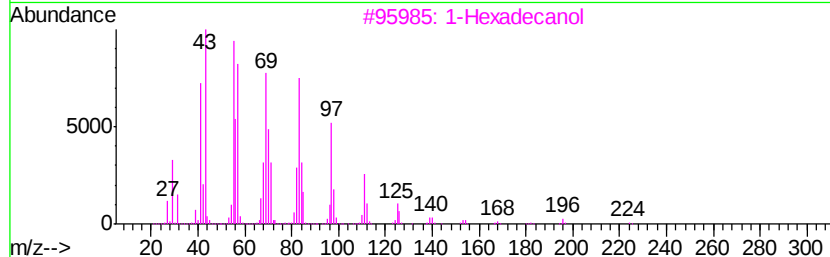
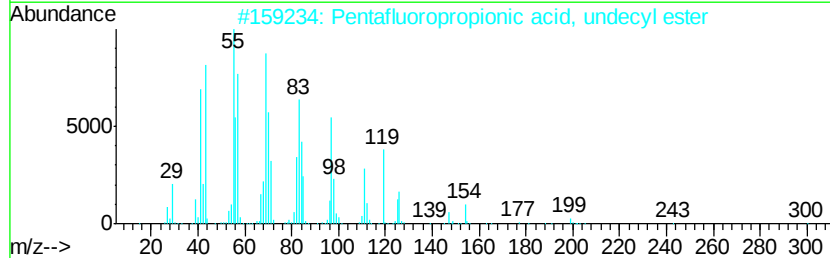
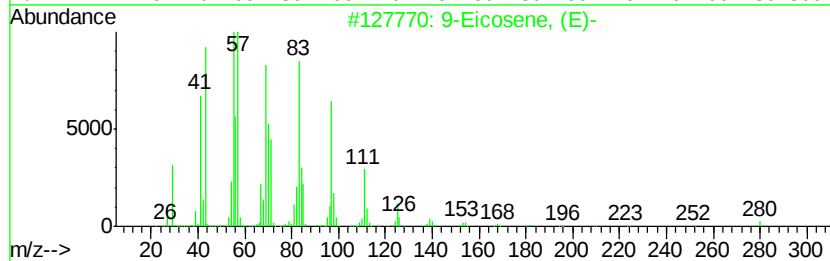
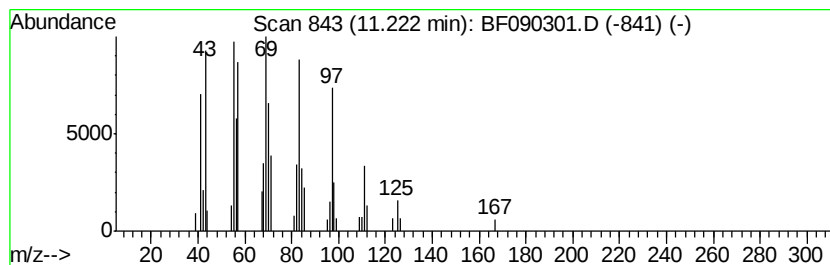
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Peak Number 6 9-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.22	2.23 ng	77974	Phenanthrene-d10	10.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
2		Pentafluoropropionic acid, undec...	318	C14H23F5O2	959014-11-0	91
3		1-Hexadecanol	242	C16H34O	036653-82-4	91
4		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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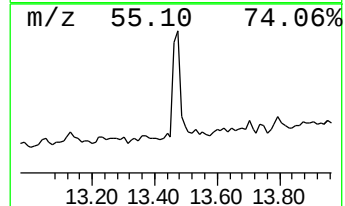
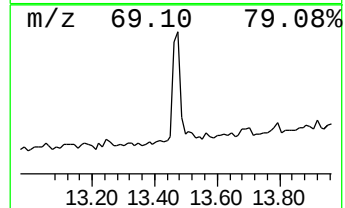
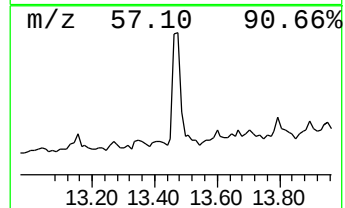
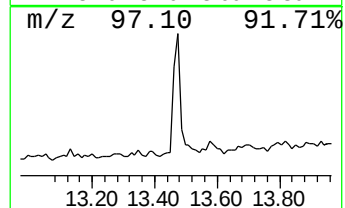
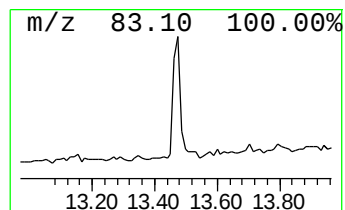
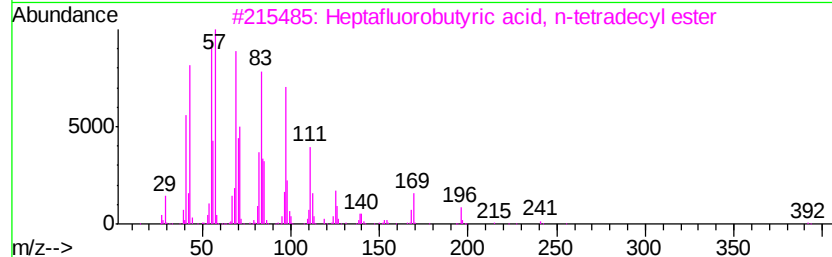
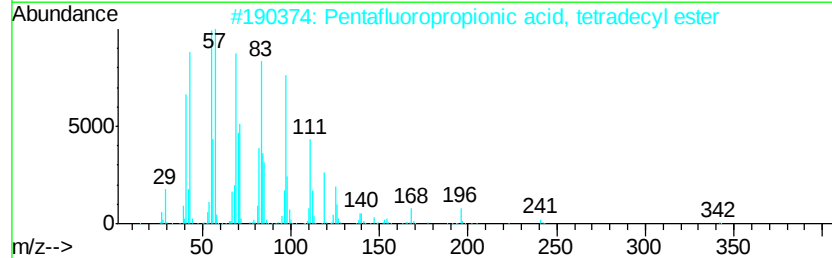
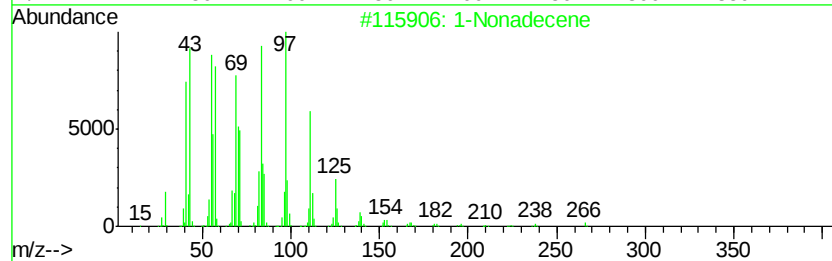
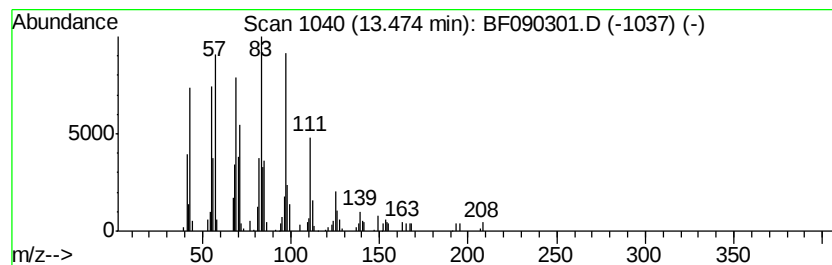
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Peak Number 7 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.47	4.81 ng	151910	Chrysene-d12	13.58	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	94
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.54	16.9	ng	553155	1	6.46	652534	20.0
unknown6.23	6.23	70.5	ng	2299030	1	6.46	652534	20.0
Heptadecane	10.43	2.4	ng	84189	4	10.97	698928	20.0
9-Eicosene, (E)-	11.22	2.2	ng	77974	4	10.97	698928	20.0
1-Nonadecene	13.47	4.8	ng	151910	5	13.58	632168	20.0