

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101416\
 Data File : BF090565.D
 Acq On : 14 Oct 2016 12:55
 Operator : UM/SJ
 Sample : H4977-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 13M

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-BF101316.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	5.114	240	243	250	rBV	738766	1111016	22.10%	2.524%
2	5.526	277	279	298	rBV	3538533	4475594	89.04%	10.168%
3	6.554	366	369	378	rBV	3669988	5026340	100.00%	11.420%
4	6.692	378	381	383	rBV	3193311	4551697	90.56%	10.341%
5	6.920	399	401	412	rBV	884293	1222569	24.32%	2.778%
6	7.069	412	414	417	rBV	2491892	3175135	63.17%	7.214%
7	7.480	447	450	456	rBV	2249587	2829051	56.28%	6.427%
8	7.572	456	458	466	rVV	102531	328247	6.53%	0.746%
9	7.686	466	468	479	rVB	32607	81045	1.61%	0.184%
10	8.200	511	513	523	rBV	1233001	1617475	32.18%	3.675%
11	9.286	605	608	610	rBV	3241393	3794197	75.49%	8.620%
12	9.400	616	618	630	rVB	63390	113769	2.26%	0.258%
13	9.675	640	642	659	rVB	1360773	1312783	26.12%	2.983%
14	9.960	664	667	679	rVB	1894996	1814798	36.11%	4.123%
15	10.749	734	736	745	rBV	2330418	2821434	56.13%	6.410%
16	10.863	745	746	753	rVB	72410	117640	2.34%	0.267%
17	11.446	795	797	810	rBV	1397579	1843212	36.67%	4.188%
18	11.675	814	817	822	rBV	266471	331752	6.60%	0.754%
19	12.498	886	889	890	rBV	166421	243294	4.84%	0.553%
20	12.909	923	925	927	rBV	62941	58414	1.16%	0.133%
21	13.035	934	936	946	rBV	3570027	4047115	80.52%	9.195%
22	13.264	954	956	959	rBV	82328	81498	1.62%	0.185%
23	13.607	984	986	989	rBV	63708	68876	1.37%	0.156%
24	13.938	1012	1015	1020	rBV2	71285	142751	2.84%	0.324%
25	14.087	1026	1028	1039	rVB	1121741	1607490	31.98%	3.652%
26	14.944	1100	1103	1107	rVB	75987	85123	1.69%	0.193%
27	15.550	1153	1156	1168	rVB	635352	1112721	22.14%	2.528%

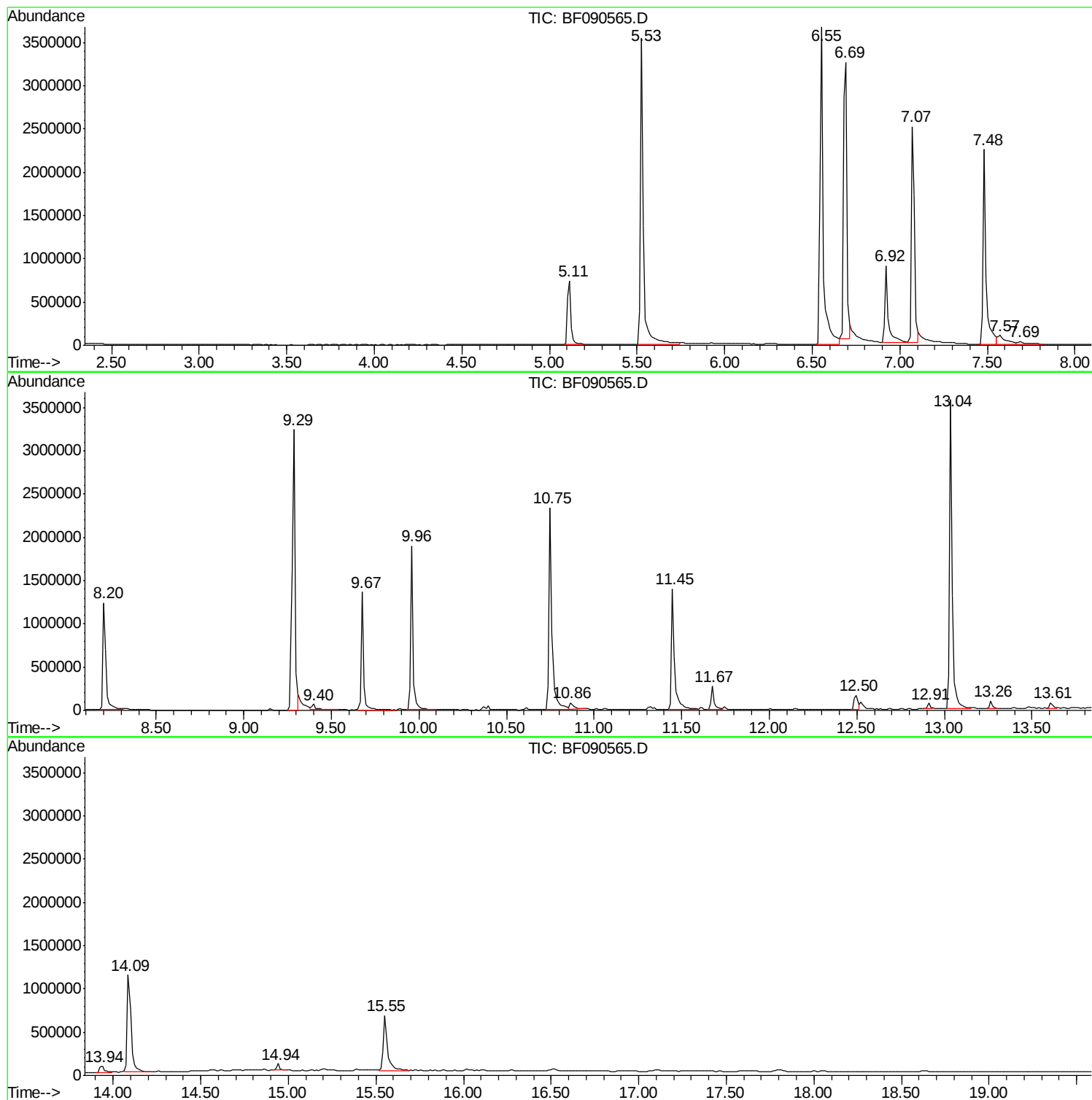
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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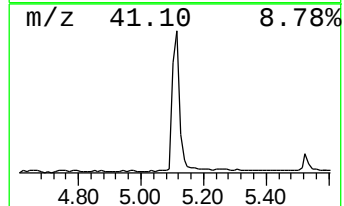
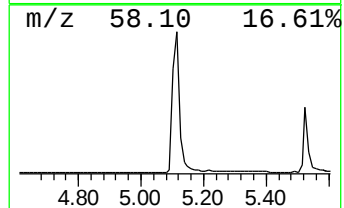
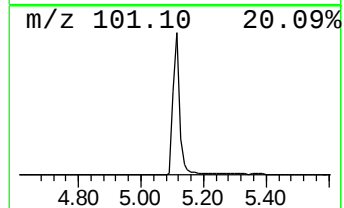
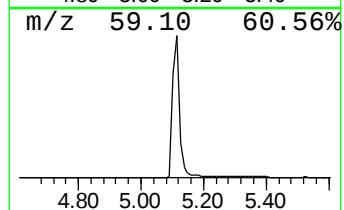
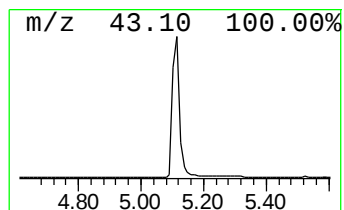
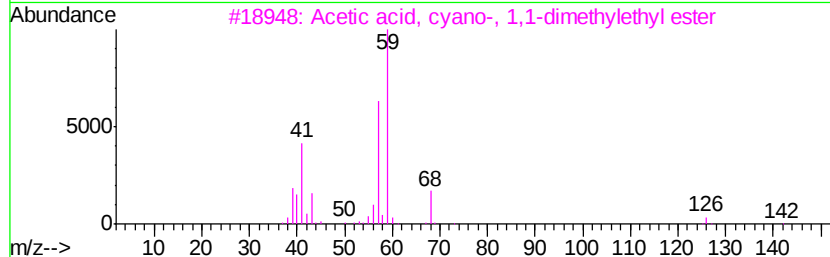
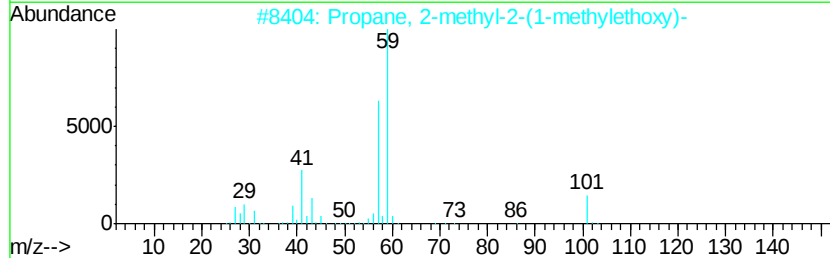
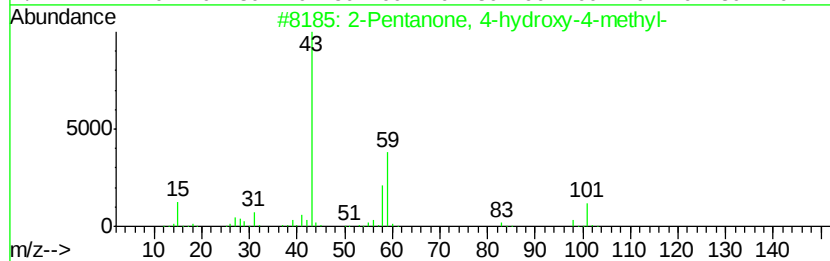
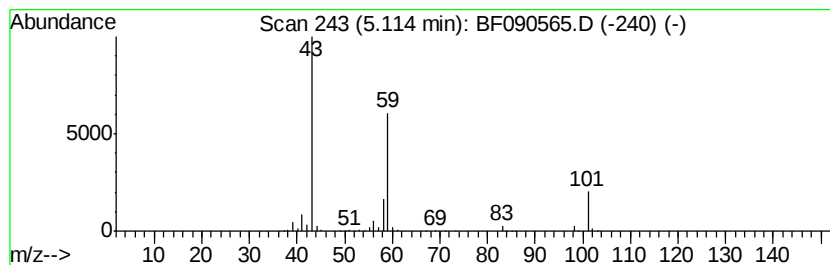
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.11	18.18 ng	1111020	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetone	58	C3H6O	000067-64-1	9



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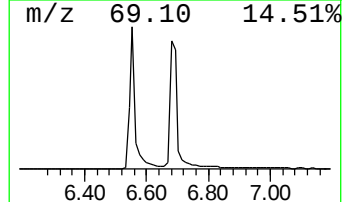
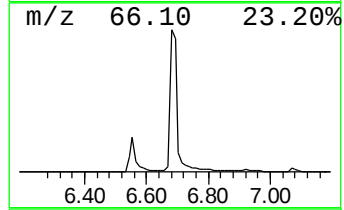
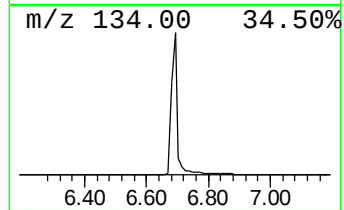
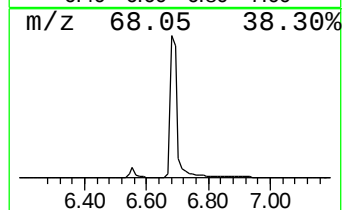
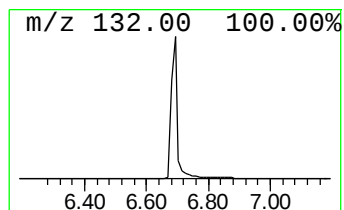
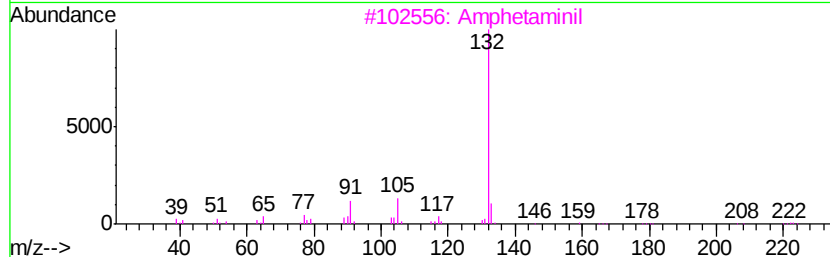
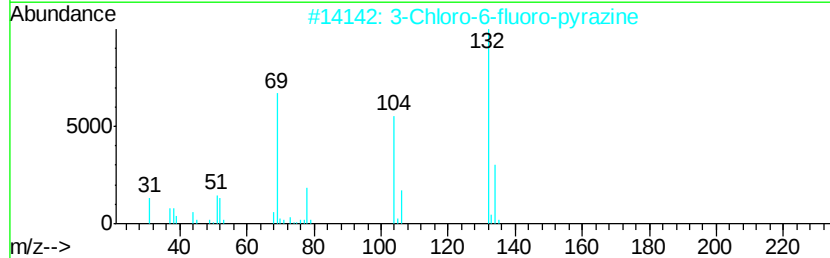
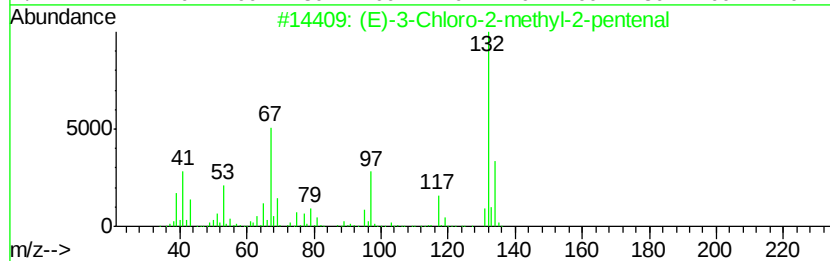
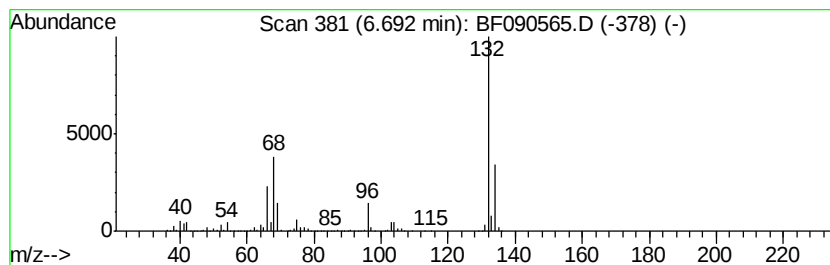
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Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	74.46 ng	4551700	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Amphetaminil	250	C17H18N2	017590-01-1	10
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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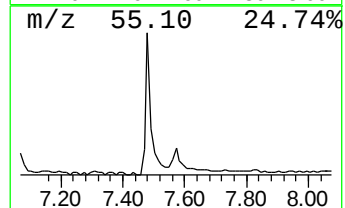
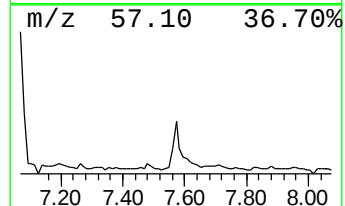
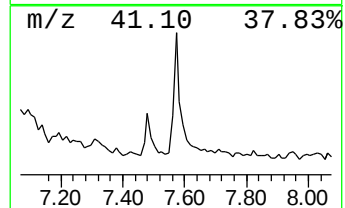
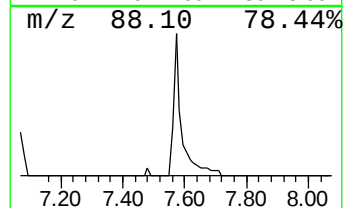
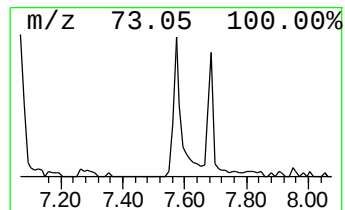
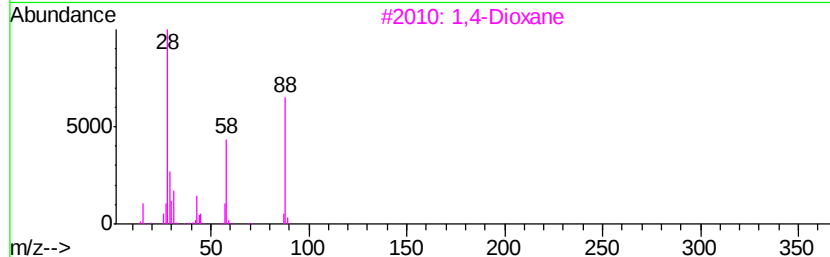
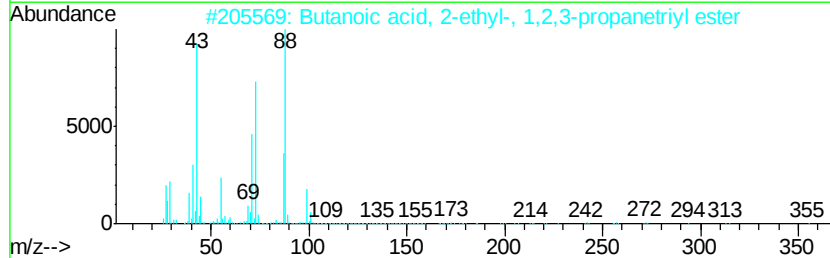
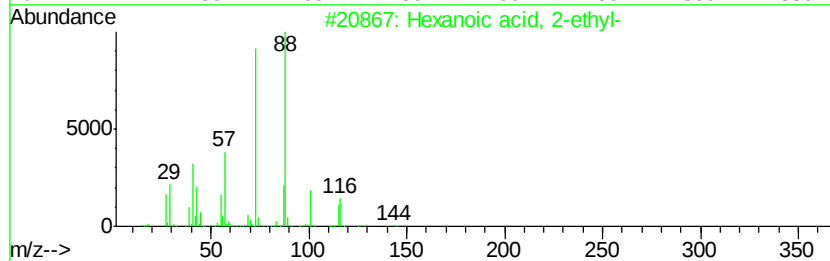
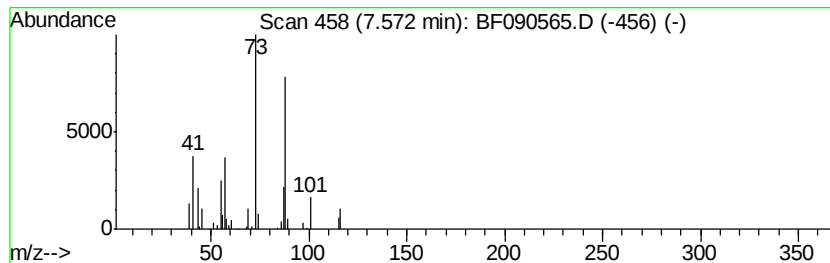
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Peak Number 4 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	4.06 ng	328247	Naphthalene-d8	8.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
2		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3		1,4-Dioxane	88	C4H8O2	000123-91-1	37
4		Hydroxypivalic acid	118	C5H10O3	004835-90-9	36
5		Methyl 4-O-acetyl-2,3-di-O-methy...	248	C11H20O6	072945-56-3	36



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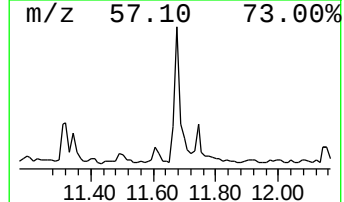
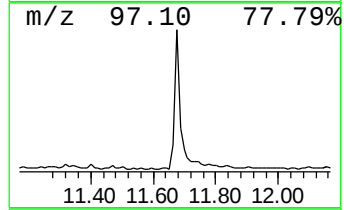
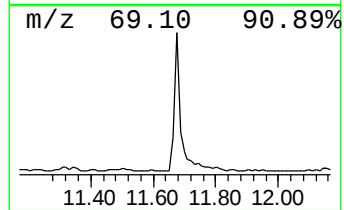
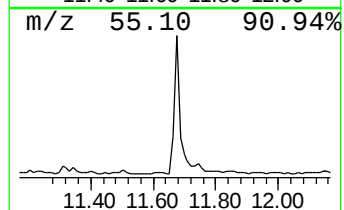
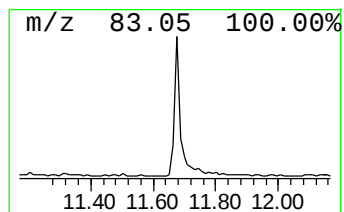
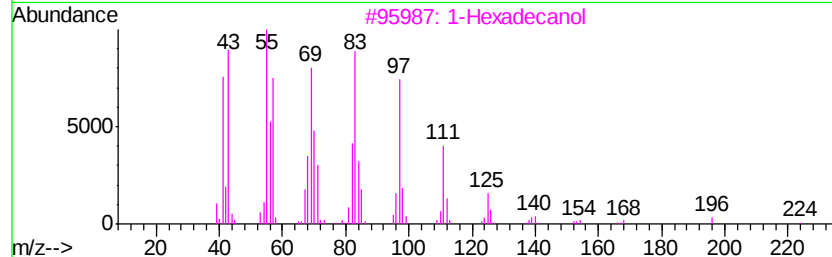
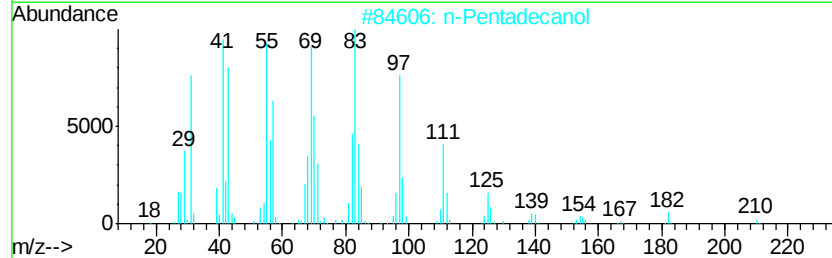
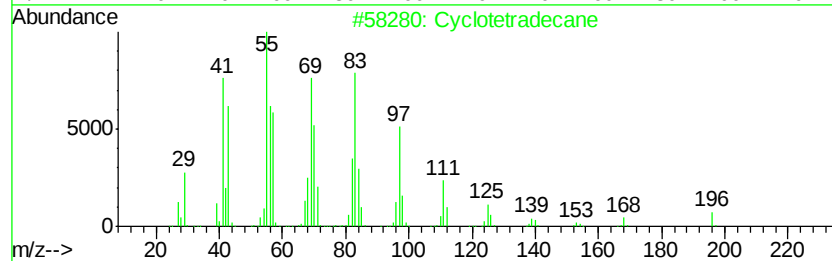
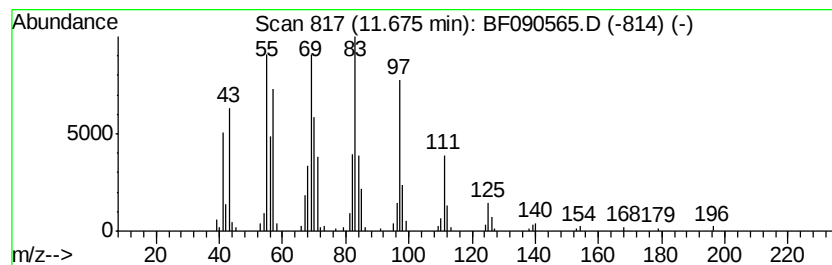
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Peak Number 5 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.67	3.60 ng	331752	Phenanthrene-d10		11.45
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvcclotetradecane	196	C14H28	000295-17-0	95
2	n-Pentadecanol	228	C15H32O	000629-76-5	94
3	1-Hexadecanol	242	C16H34O	036653-82-4	94
4	2-Tetradecene, (E)-	196	C14H28	035953-54-9	92
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91



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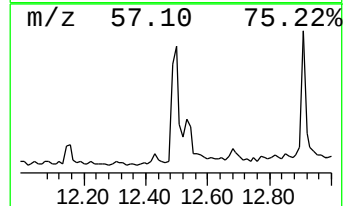
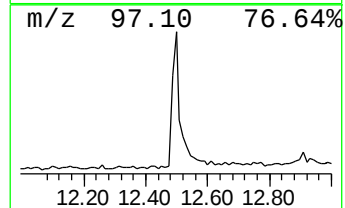
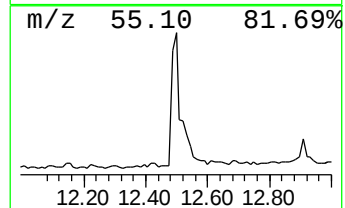
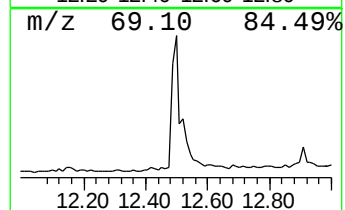
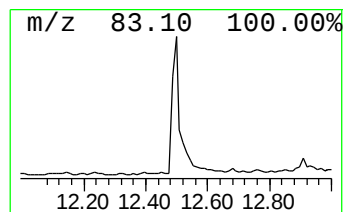
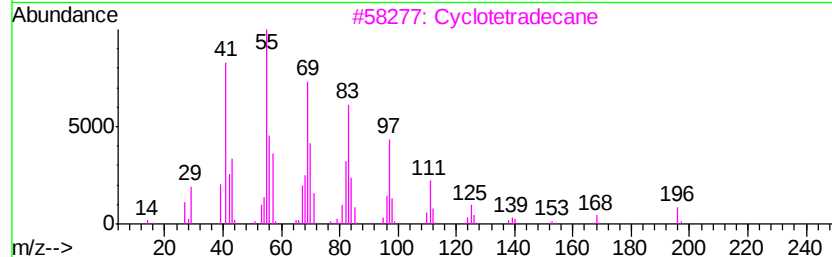
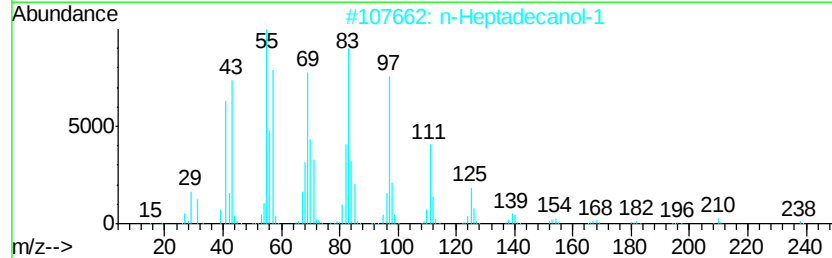
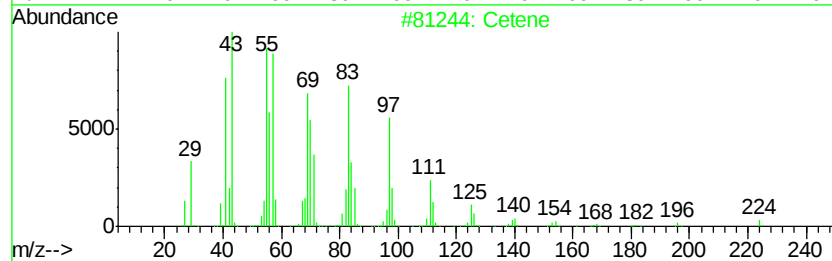
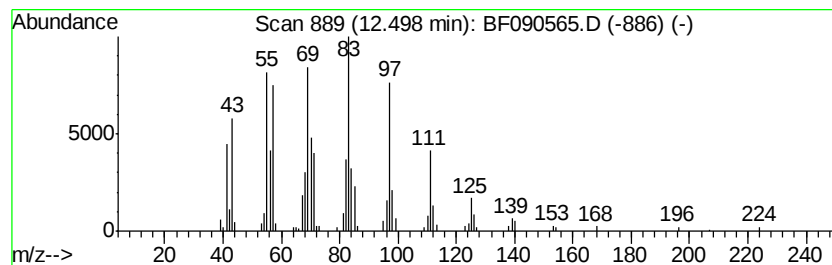
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Peak Number 6 Cetene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	2.64 ng	243294	Phenanthrene-d10	11.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cetene	224	C16H32	000629-73-2	96
2		n-Heptadecanol-1	256	C17H36O	001454-85-9	95
3		Cyclotetradecane	196	C14H28	000295-17-0	94
4		Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	94
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.11	18.2	ng	1111020	1	6.92	1222570	20.0
unknown6.69	6.69	74.5	ng	4551700	1	6.92	1222570	20.0
Hexanoic acid, 2-...	7.57	4.1	ng	328247	2	8.20	1617480	20.0
Cyclotetradecane	11.67	3.6	ng	331752	4	11.45	1843210	20.0
Cetene	12.50	2.6	ng	243294	4	11.45	1843210	20.0