

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080316\
 Data File : BF089586.D
 Acq On : 4 Aug 2016 12:23
 Operator : UM/SJ
 Sample : H4321-03
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3-PAH

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-BF080316.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	4.684	268	271	288	rBV	99670	221328	19.97%	2.784%
2	5.359	328	330	355	rBV	444305	882711	79.63%	11.101%
3	7.005	471	474	481	rBV	462653	875500	78.98%	11.011%
4	7.107	481	483	508	rVV	602906	1108504	100.00%	13.941%
5	7.462	512	514	529	rVV	128811	219078	19.76%	2.755%
6	7.702	532	535	552	rVB	445003	715681	64.56%	9.001%
7	8.365	591	593	621	rBV	302818	568274	51.26%	7.147%
8	9.485	689	691	710	rBV	186553	302718	27.31%	3.807%
9	11.268	844	847	876	rBV	706313	897673	80.98%	11.290%
10	11.954	905	907	916	rBV	91075	117348	10.59%	1.476%
11	12.308	936	938	946	rBV	216184	312189	28.16%	3.926%
12	13.177	1011	1014	1016	rBB	9906	13920	1.26%	0.175%
13	13.600	1049	1051	1061	rBV	309558	432137	38.98%	5.435%
14	13.942	1079	1081	1088	rBB	14764	23185	2.09%	0.292%
15	14.708	1146	1148	1158	rVB	154160	216581	19.54%	2.724%
16	15.714	1234	1236	1240	rBB	9275	12143	1.10%	0.153%
17	17.063	1352	1354	1369	rBV	365231	440845	39.77%	5.544%
18	18.331	1463	1465	1469	rBV	14141	26456	2.39%	0.333%
19	18.400	1469	1471	1477	rBV	162716	207685	18.74%	2.612%
20	19.566	1570	1573	1575	rBV	10931	15529	1.40%	0.195%
21	19.852	1595	1598	1599	rBV	10610	13522	1.22%	0.170%
22	20.069	1614	1617	1625	rBV	140460	236188	21.31%	2.970%
23	20.343	1639	1641	1644	rBV	8561	12902	1.16%	0.162%
24	20.537	1655	1658	1660	rVB	9559	12481	1.13%	0.157%
25	20.583	1660	1662	1664	rBV3	6734	13143	1.19%	0.165%
26	20.926	1689	1692	1697	rBV3	8050	20006	1.80%	0.252%
27	21.463	1736	1739	1742	rBV3	6024	14327	1.29%	0.180%
28	22.092	1788	1794	1800	rVB7	4320	19238	1.74%	0.242%

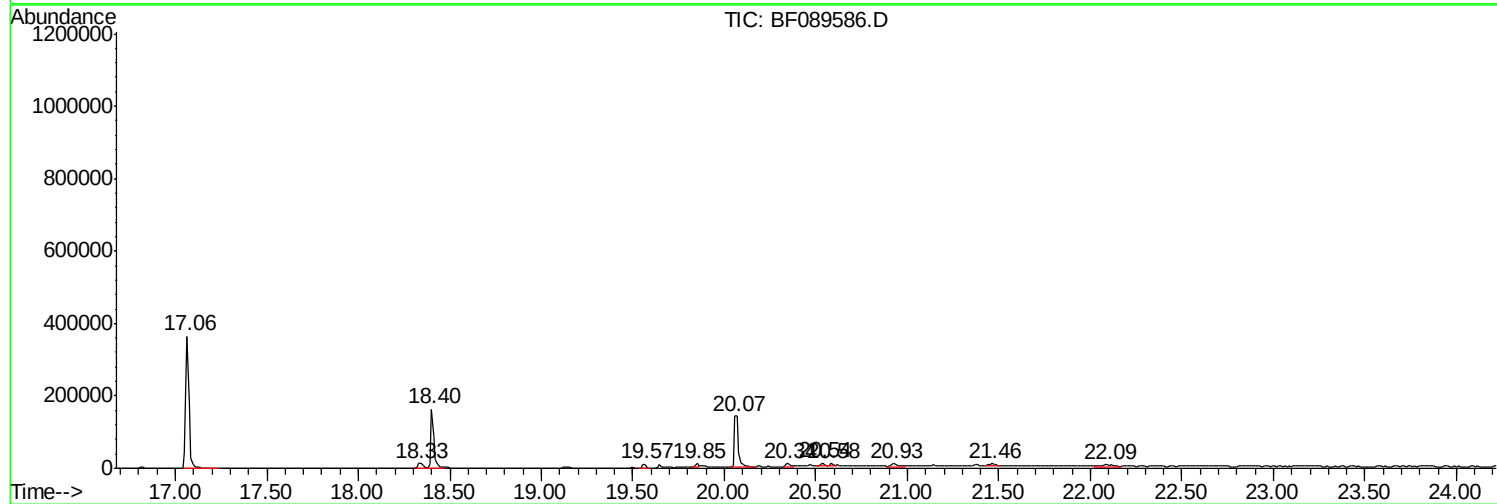
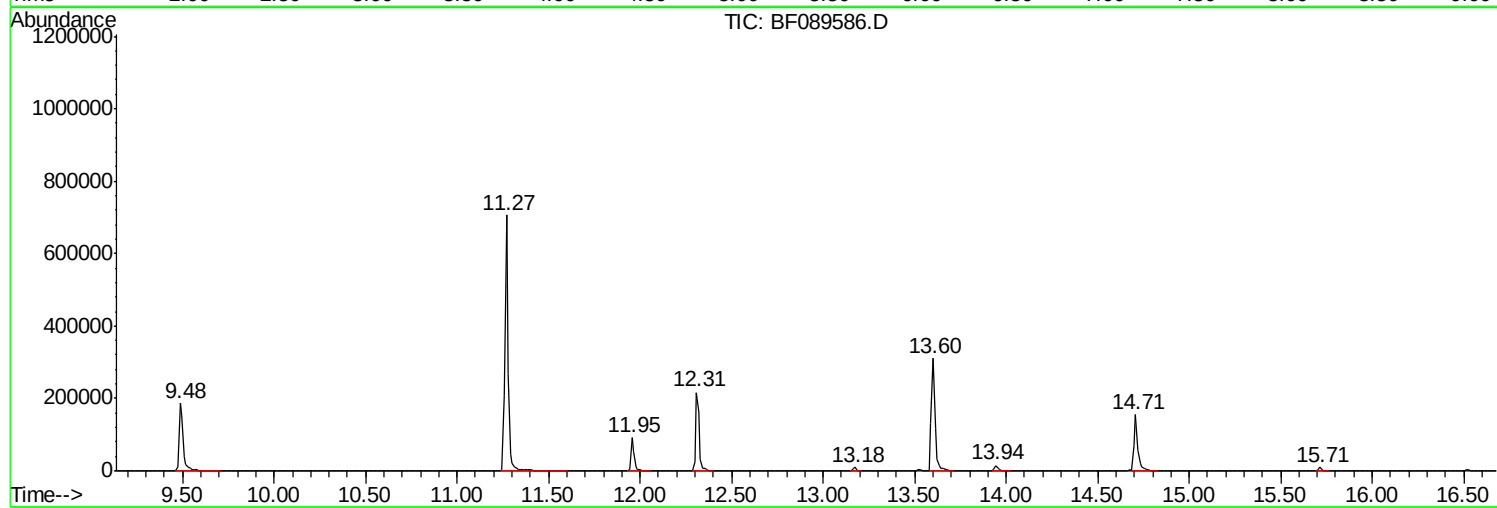
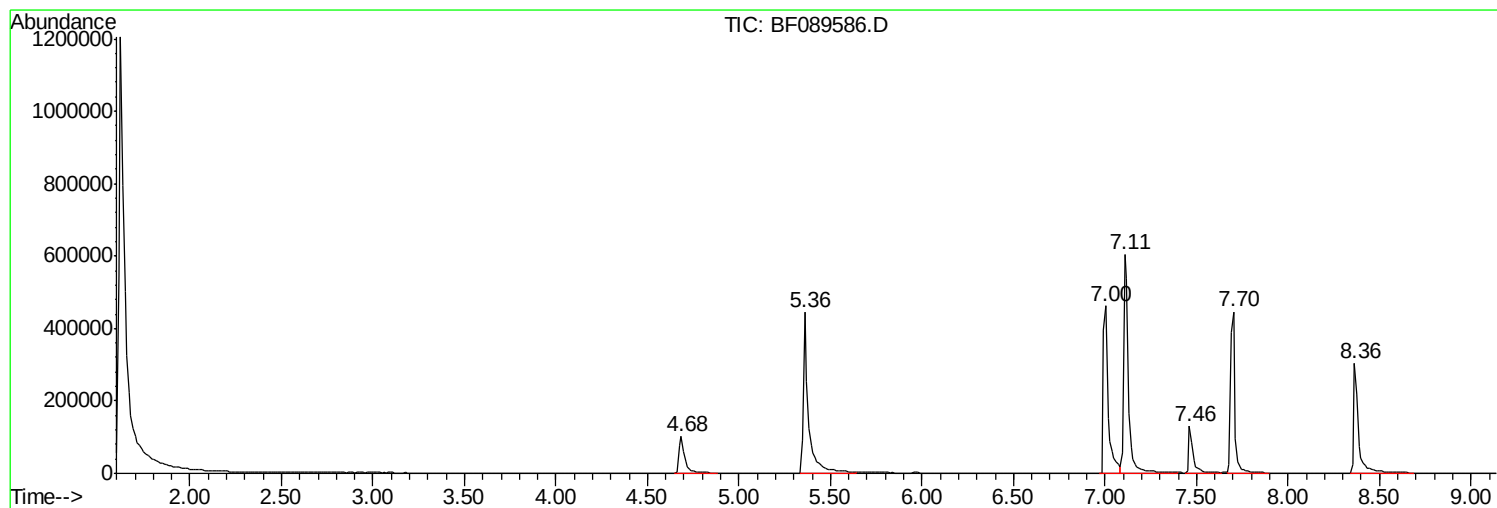
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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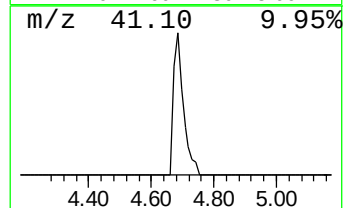
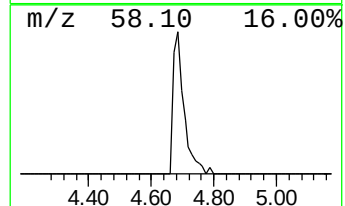
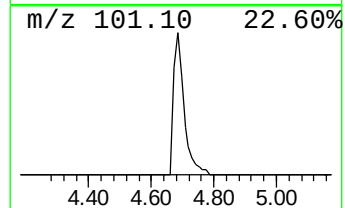
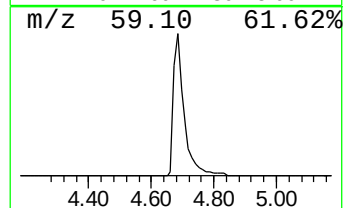
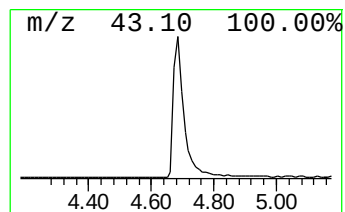
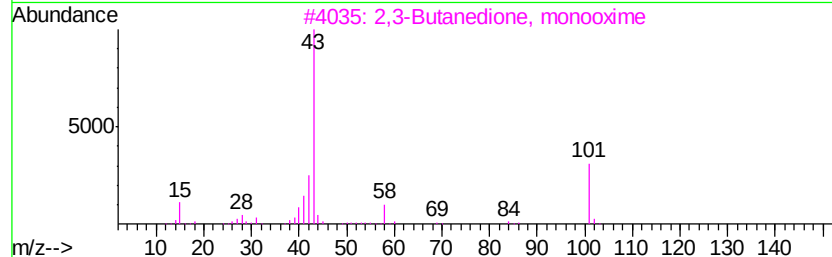
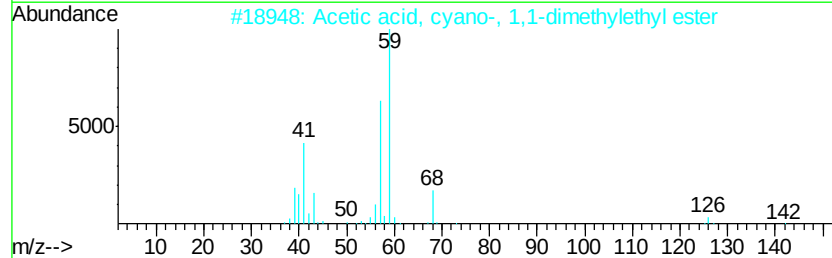
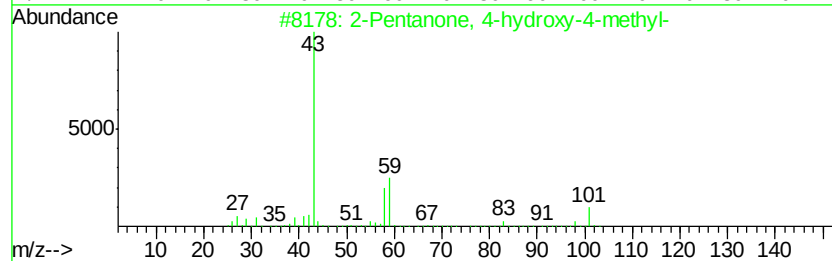
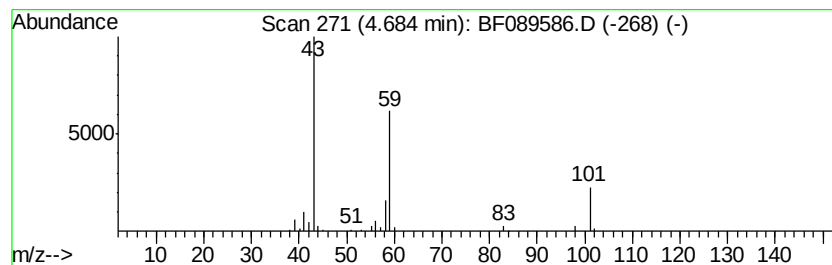
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.68	20.21 ng	221328	1,4-Dichlorobenzene-d4	7.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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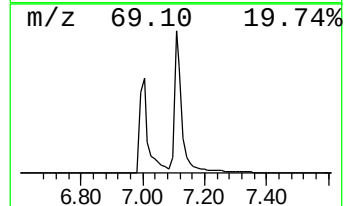
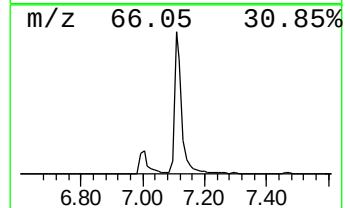
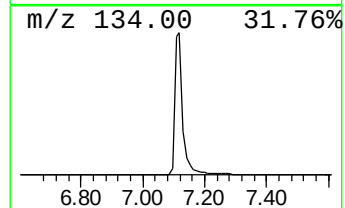
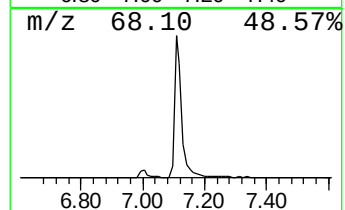
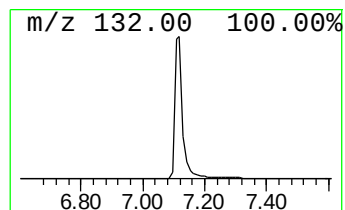
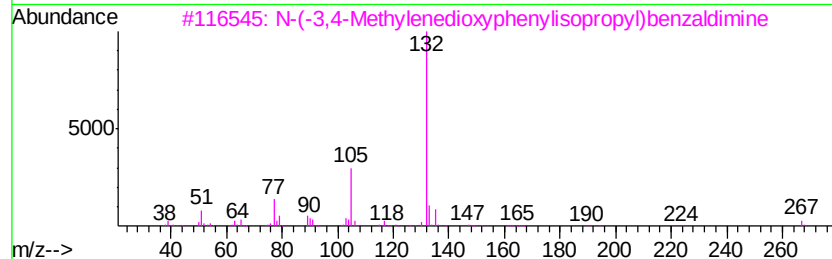
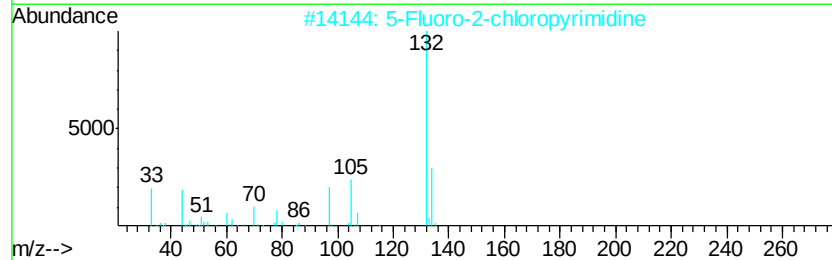
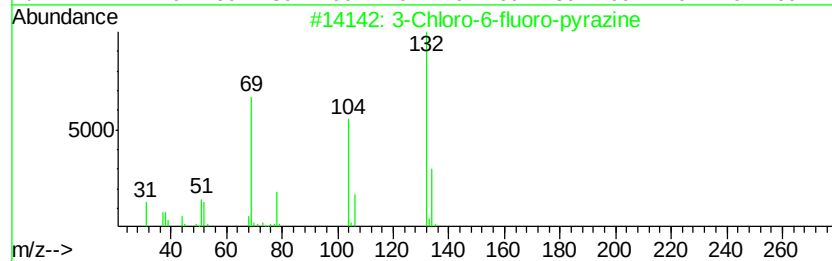
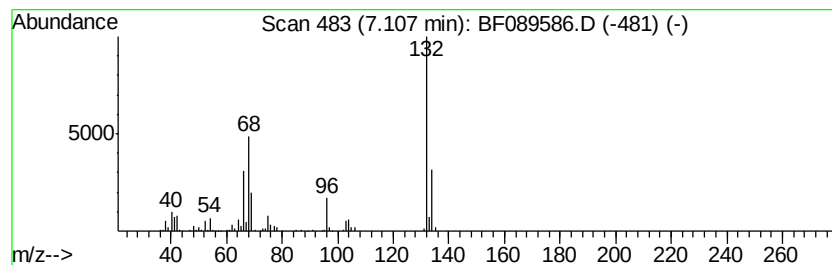
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Peak Number 2 unknown7.11 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.11	101.20 ng	1108500	1,4-Dichlorobenzene-d4	7.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		N-(-3,4-Methylenedioxyphenylisopropyl)-	267	C17H17NO2	1000378-96-6	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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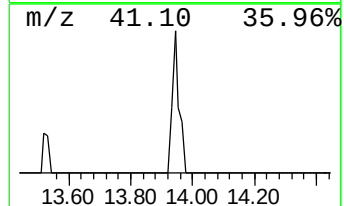
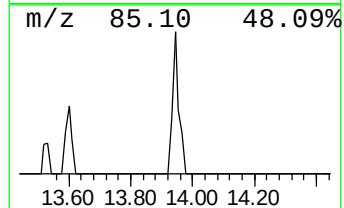
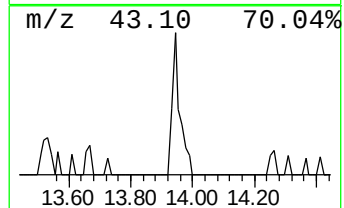
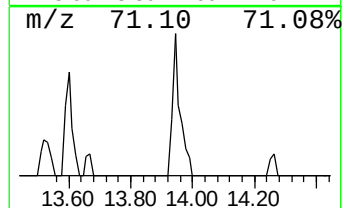
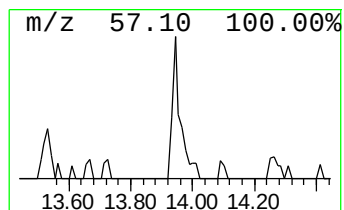
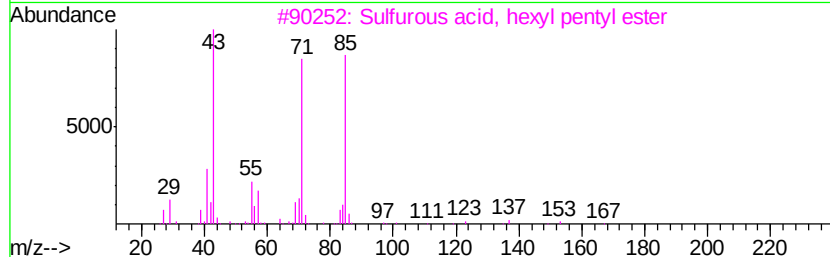
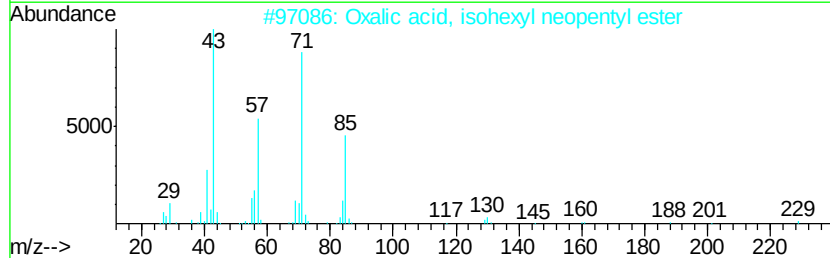
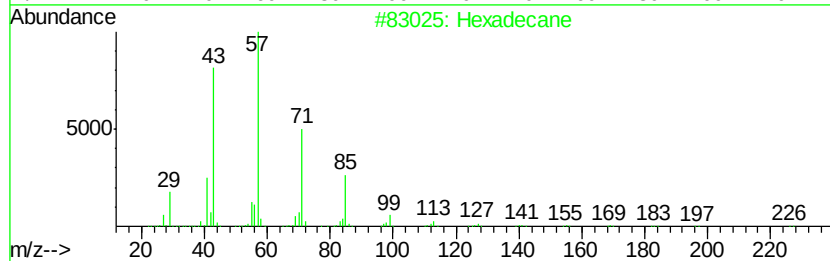
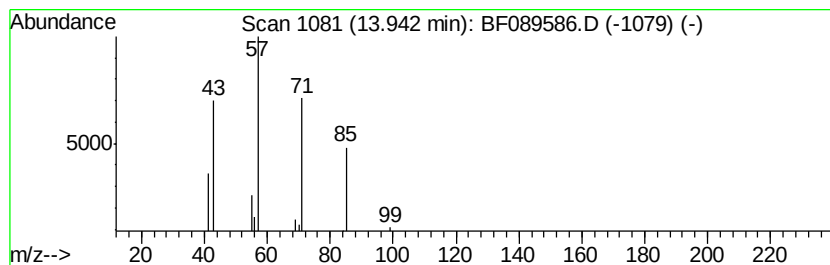
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Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.14 ng	23185	Phenanthrene-d10	14.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	74
2	Oxalic acid, isohexyl neopentyl ...		244	C13H24O4	1000309-73-0	72
3	Sulfurous acid, hexyl pentyl ester		236	C11H24O3S	1000309-14-1	56
4	Hexane, 2,2,3,3-tetramethyl-		142	C10H22	013475-81-5	50
5	Sulfurous acid, hexyl heptyl ester		264	C13H28O3S	1000309-12-9	42



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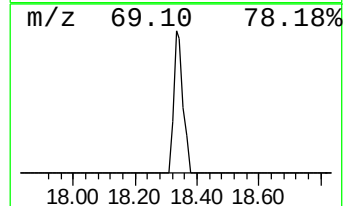
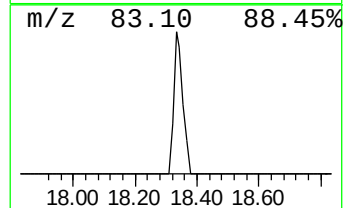
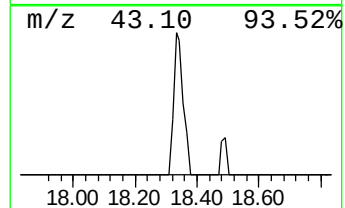
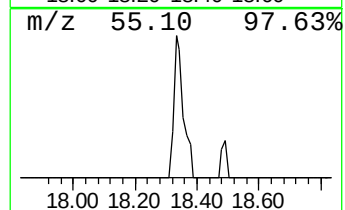
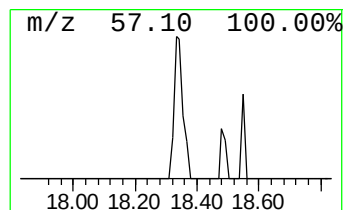
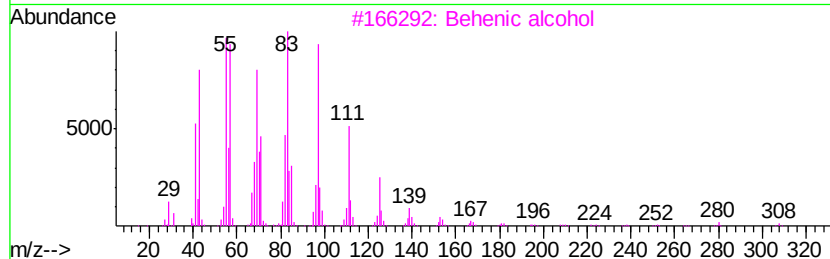
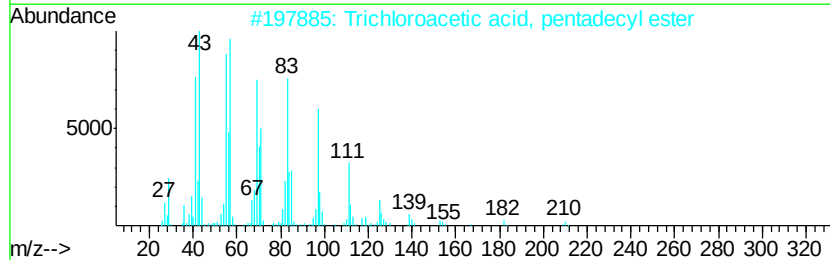
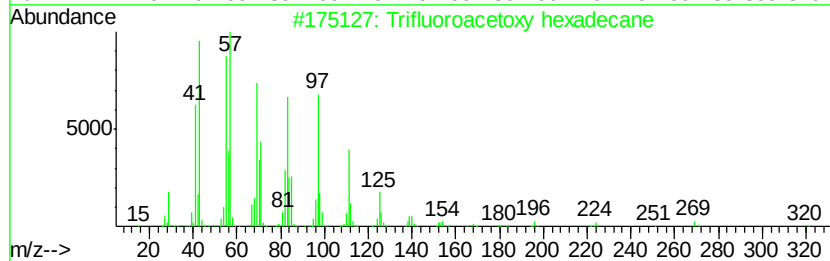
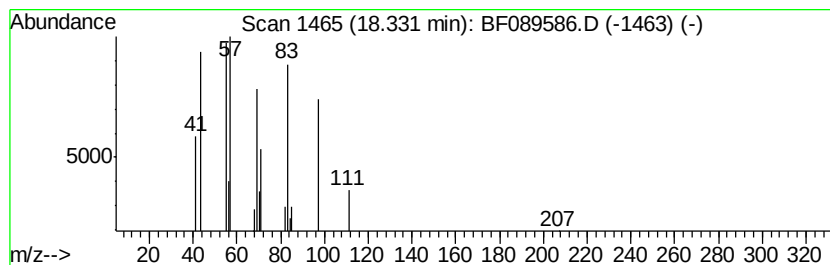
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.33	2.55 ng	26456	Chrysene-d12	18.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		Behenic alcohol	326	C22H46O	000661-19-8	87
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	20.2	ng	221328	1	7.46	219078	20.0
unknown7.11	7.11	101.2	ng	1108500	1	7.46	219078	20.0
Hexadecane	13.94	2.1	ng	23185	4	14.71	216581	20.0
Trifluoroacetoxy ...	18.33	2.5	ng	26456	5	18.40	207685	20.0