

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081916\
 Data File : BF089818.D
 Acq On : 20 Aug 2016 1:19
 Operator : UM/SJ
 Sample : H4518-17
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-1-2(5-15)

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-BF081916.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	1.655	5	6	15	rBV	2720150	5037903	21.32%	3.497%
2	1.781	15	17	25	rBV	10759741	23627761	100.00%	16.399%
3	4.833	281	284	292	rBV	2801004	4258192	18.02%	2.955%
4	5.279	319	323	325	rBV	8689233	13444111	56.90%	9.331%
5	5.679	356	358	361	rBV	244112	271336	1.15%	0.188%
6	6.330	411	415	417	rBV	10485598	13324622	56.39%	9.248%
7	6.456	423	426	428	rBV	11186434	13681277	57.90%	9.496%
8	6.684	444	446	448	rBV	3923039	3150595	13.33%	2.187%
9	6.844	457	460	462	rVB	10823617	10569390	44.73%	7.336%
10	7.096	481	482	485	rVB	358340	316224	1.34%	0.219%
11	7.256	492	496	498	rBV	6991545	8659870	36.65%	6.011%
12	7.964	556	558	560	rBV	3638157	3651709	15.46%	2.535%
13	9.050	650	653	655	rBV	13843831	12934442	54.74%	8.977%
14	9.439	685	687	690	rBV	2107989	2453527	10.38%	1.703%
15	9.713	709	711	714	rBV	4426788	3931017	16.64%	2.728%
16	10.502	777	780	782	rBV	6336143	6658793	28.18%	4.622%
17	10.639	790	792	799	rVB	286014	337350	1.43%	0.234%
18	11.188	838	840	843	rBV	3630193	3274262	13.86%	2.273%
19	11.736	886	888	900	rBV3	204213	365168	1.55%	0.253%
20	12.776	977	979	982	rBV	6868392	7731776	32.72%	5.366%
21	13.725	1060	1062	1068	rBV	214666	429318	1.82%	0.298%
22	13.839	1070	1072	1075	rBV	2948704	2818921	11.93%	1.957%
23	15.302	1198	1200	1203	rBV	2183280	3150950	13.34%	2.187%

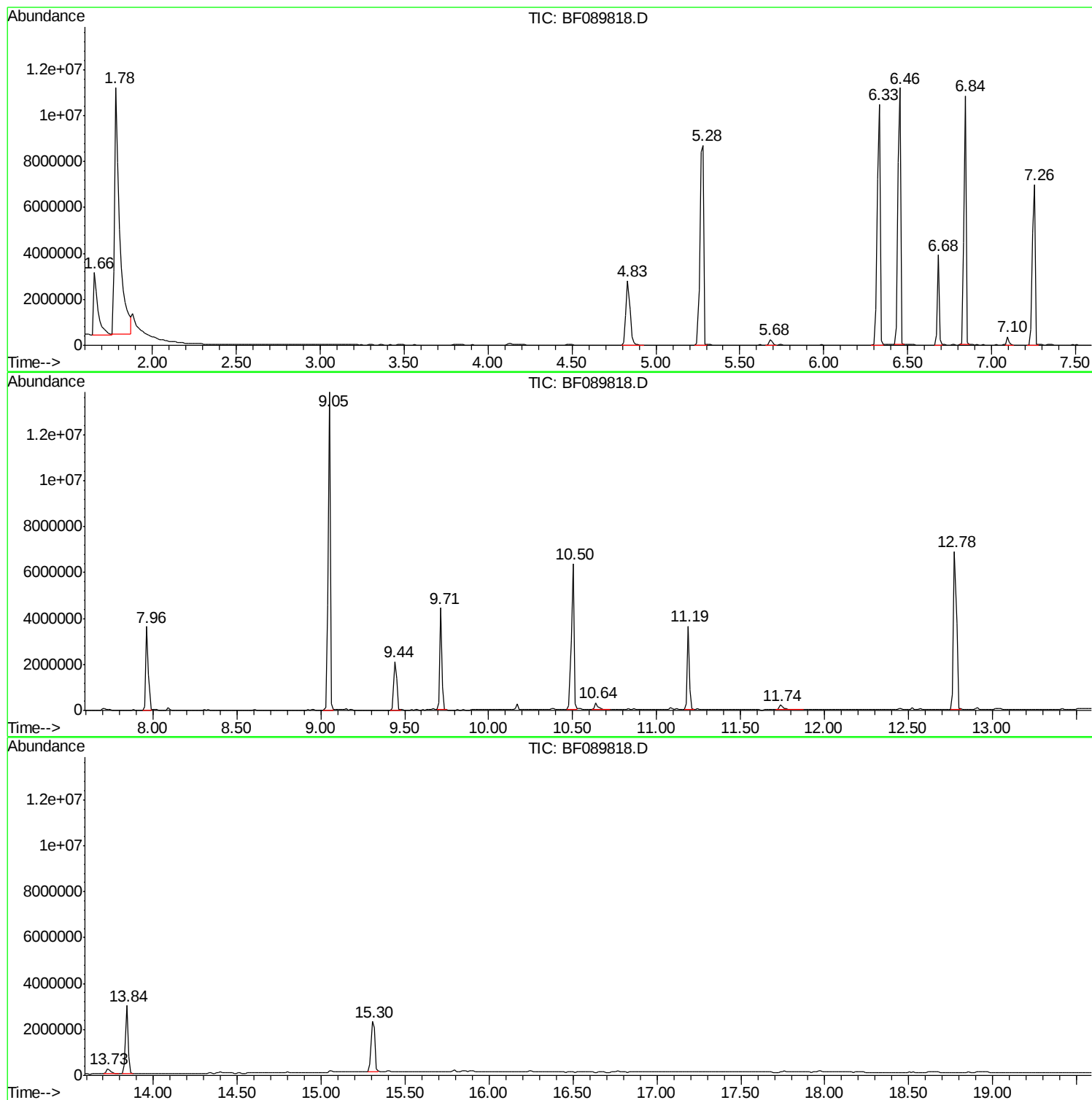
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ClientSampled :
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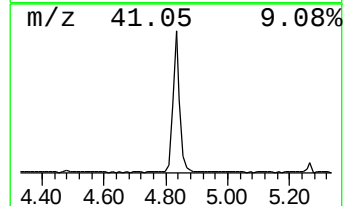
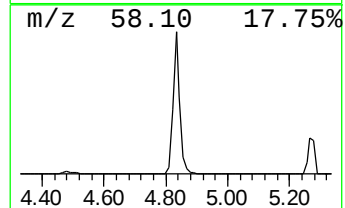
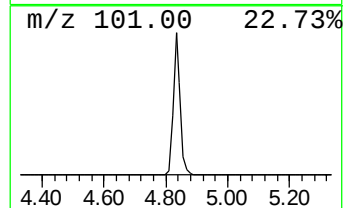
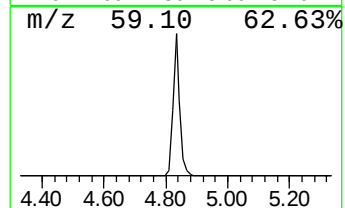
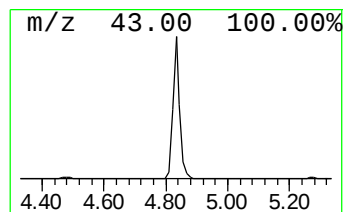
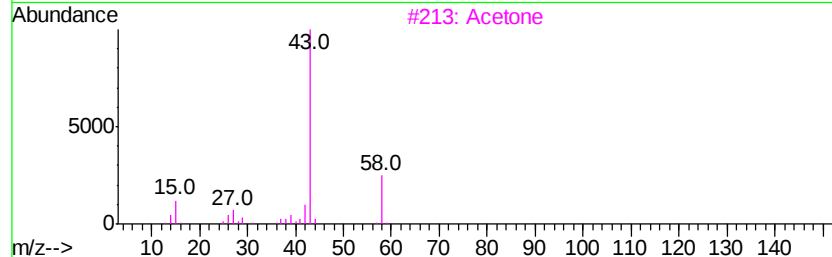
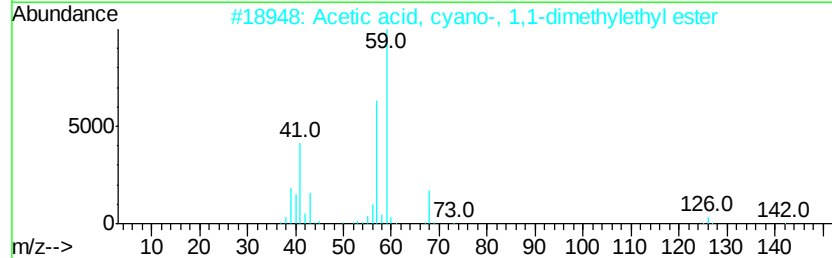
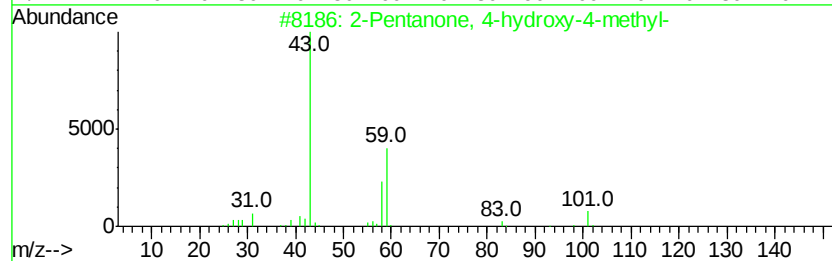
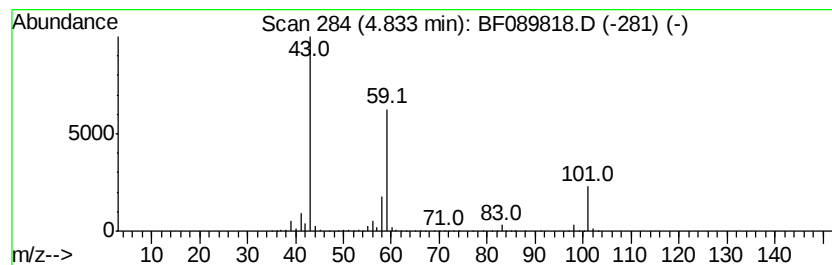
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	27.03 ng	4258190	1,4-Dichlorobenzene-d4	6.68

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		Acetone	58	C3H6O	000067-64-1	9
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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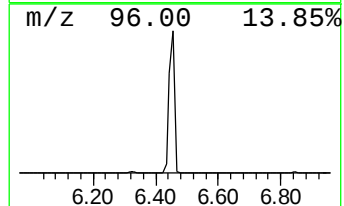
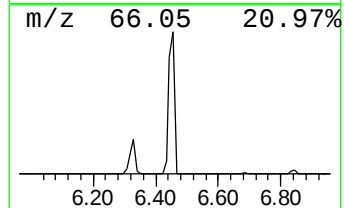
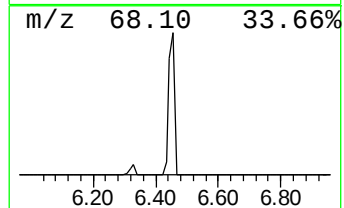
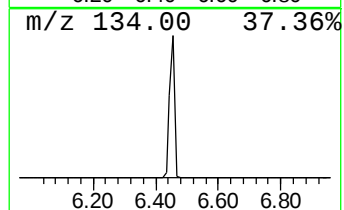
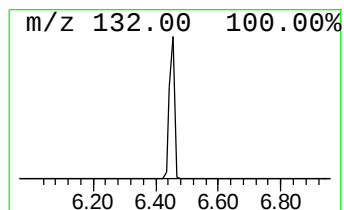
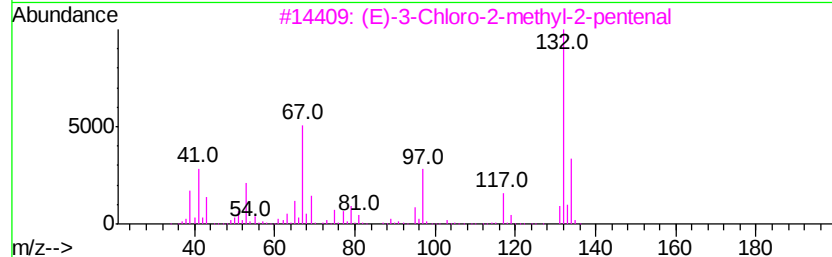
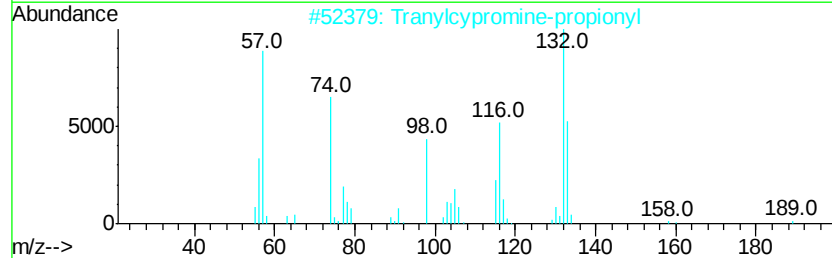
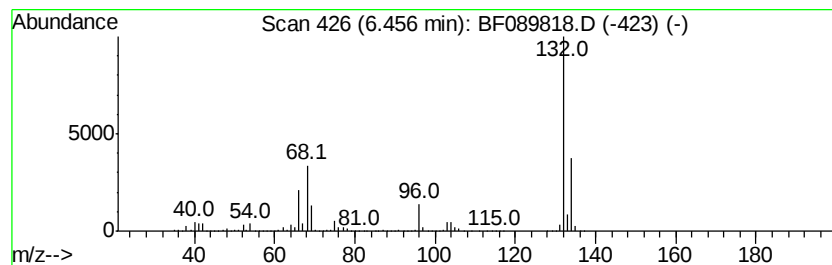
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Peak Number 4 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	86.85 ng	13681300	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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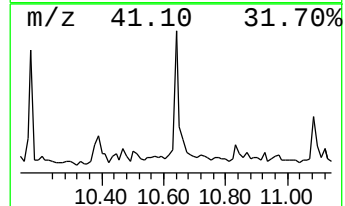
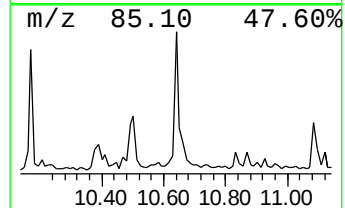
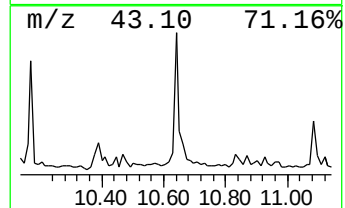
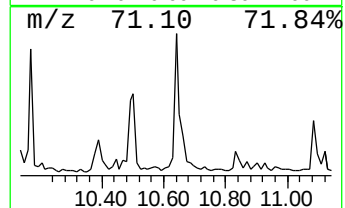
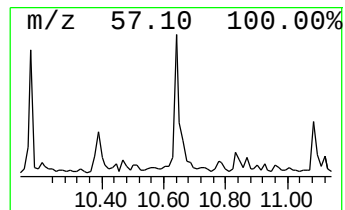
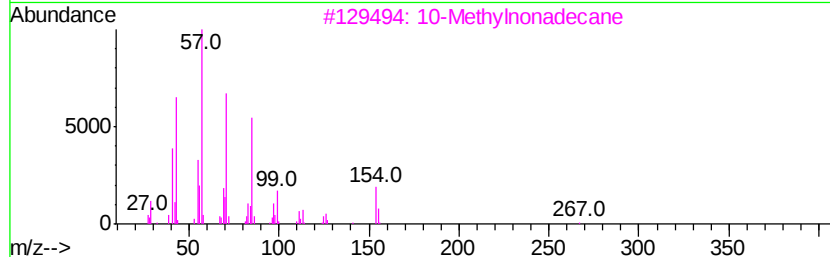
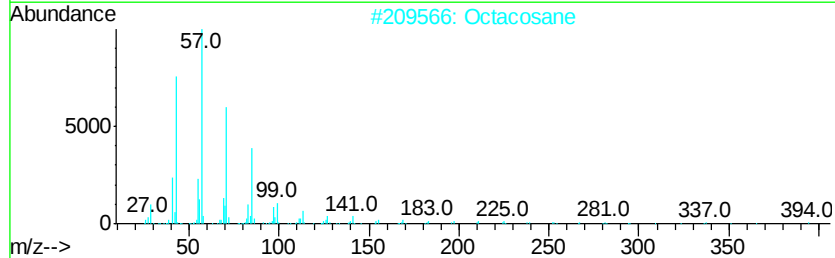
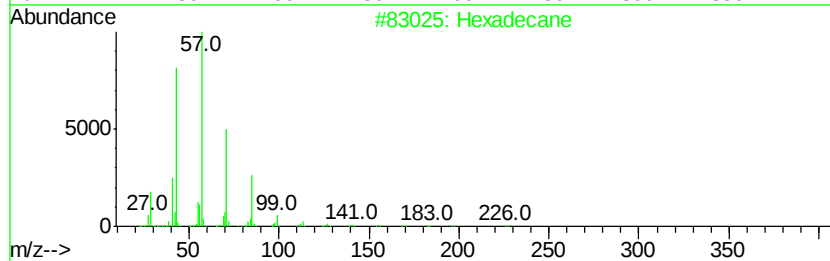
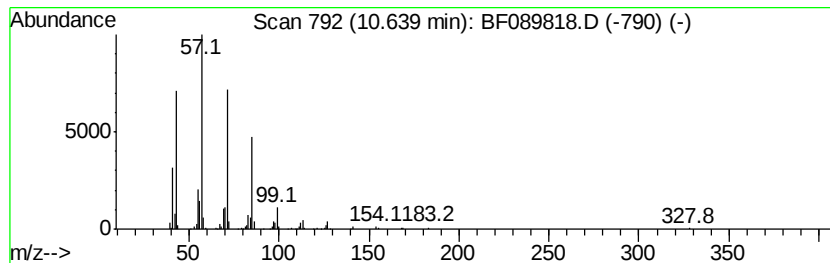
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Peak Number 6 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.64	2.06 ng	337350	Phenanthrene-d10	11.19		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	80
2	Octacosane		394	C28H58	000630-02-4	78
3	10-Methylnonadecane		282	C20H42	056862-62-5	72
4	Nonadecane		268	C19H40	000629-92-5	64
5	1,3-Dimethylcyclopentanol		114	C7H14O	019550-46-0	64



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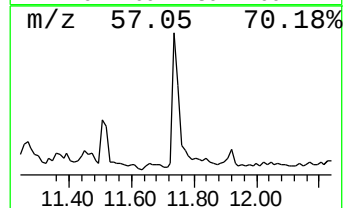
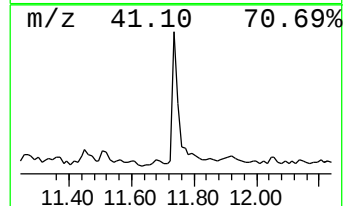
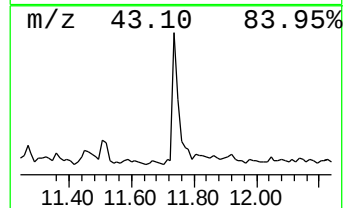
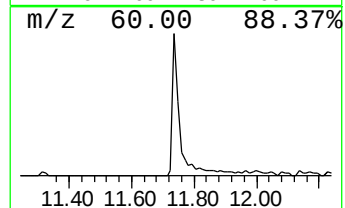
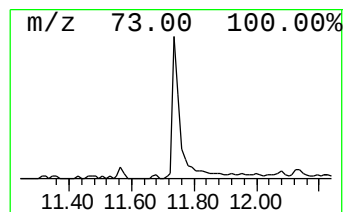
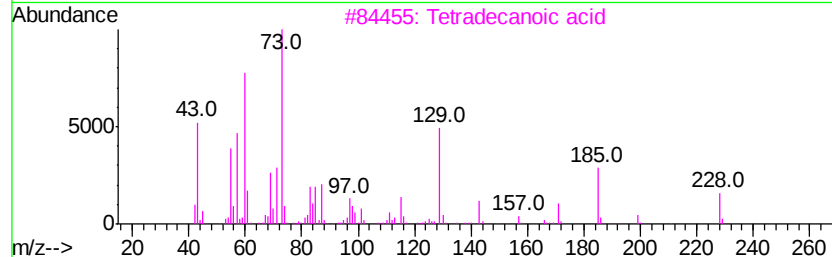
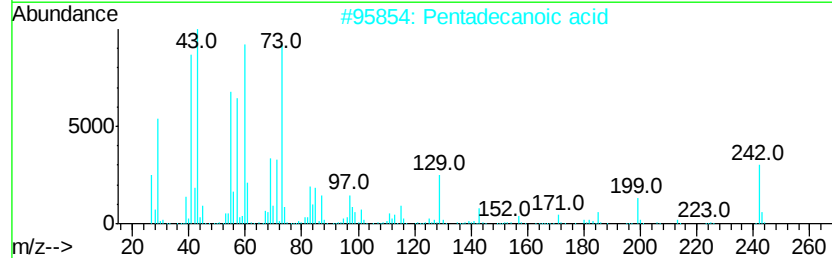
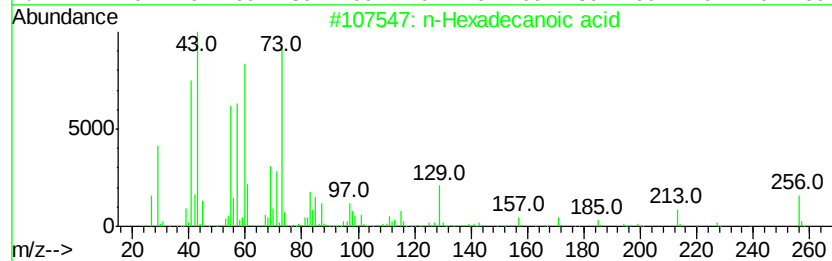
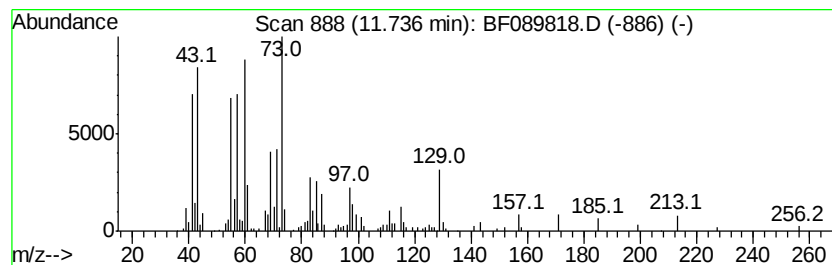
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	2.23 ng	365168	Phenanthrene-d10	11.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	38
5		Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	30



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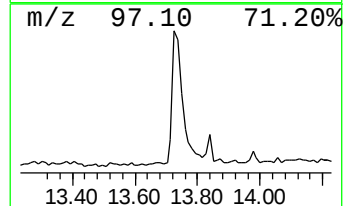
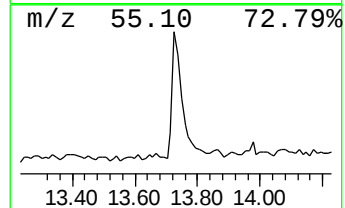
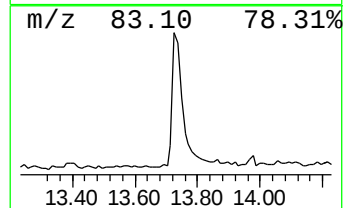
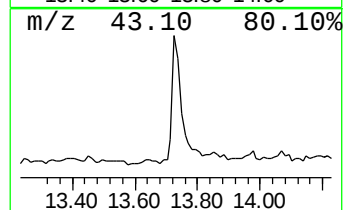
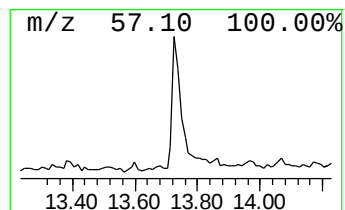
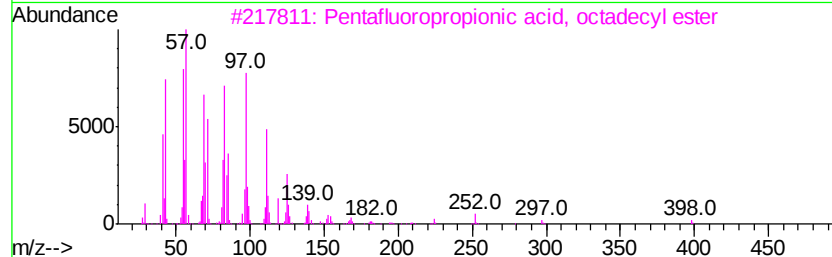
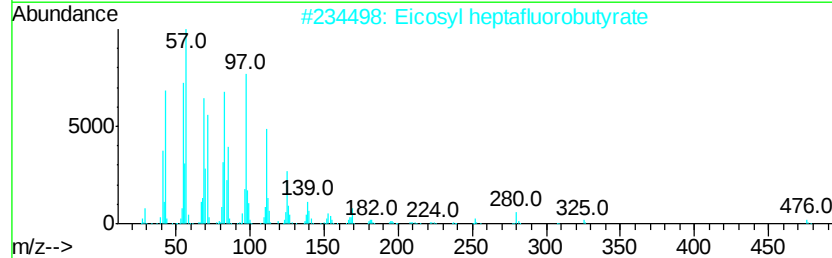
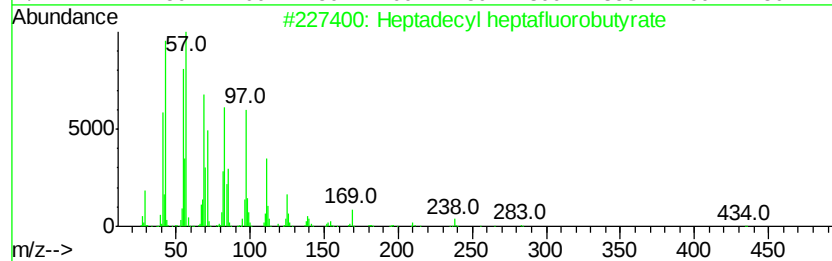
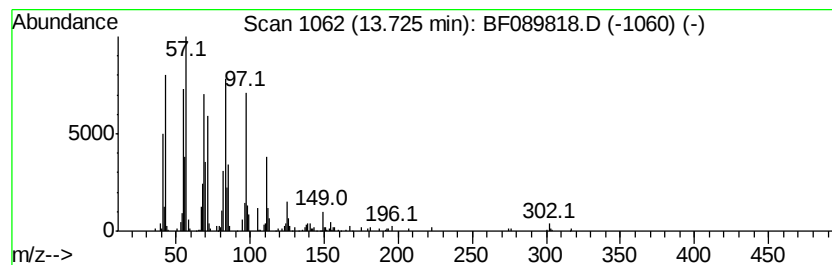
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Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	3.05 ng	429318	Chrysene-d12	13.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	90
3			Pentafluoropropionic acid, octadec...	416	C21H37F5O2	959261-25-7	90
4			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	90
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.46	6.46	86.8	ng	13681300	1	6.68	3150600	20.0
Hexadecane	10.64	2.1	ng	337350	4	11.19	3274260	20.0
n-Hexadecanoic acid	11.74	2.2	ng	365168	4	11.19	3274260	20.0
Heptadecyl heptaf...	13.73	3.0	ng	429318	5	13.84	2818920	20.0