

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
 Data File : BF088080.D
 Acq On : 16 Jun 2016 17:22
 Operator : UM/SJ
 Sample : H3570-18
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-20-COMP

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-BF060716.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	1.678	7	8	17	rVB	261530	490701	18.52%	2.535%
2	1.804	17	19	26	rBV	1652856	2649610	100.00%	13.689%
3	4.878	286	288	297	rBV	65888	107283	4.05%	0.554%
4	5.301	323	325	328	rBV	1268795	1441588	54.41%	7.448%
5	6.364	415	418	420	rBV	1168179	1592969	60.12%	8.230%
6	6.479	426	428	431	rBV	1228902	1550974	58.54%	8.013%
7	6.719	446	449	451	rBV	716139	614820	23.20%	3.177%
8	6.867	460	462	465	rBV	1003810	1227237	46.32%	6.341%
9	7.279	496	498	501	rBV	730715	981801	37.05%	5.073%
10	7.999	559	561	564	rBV	777542	791015	29.85%	4.087%
11	9.085	653	656	658	rBV	1476337	1692304	63.87%	8.743%
12	9.473	688	690	692	rVB	400746	402269	15.18%	2.078%
13	9.690	707	709	712	rBV	24201	27218	1.03%	0.141%
14	9.748	712	714	717	rVB	771544	869469	32.81%	4.492%
15	10.193	751	753	755	rVB	72573	54102	2.04%	0.280%
16	10.410	769	772	775	rBV	20897	33592	1.27%	0.174%
17	10.536	781	783	786	rBV	1044875	952333	35.94%	4.920%
18	10.662	792	794	799	rBV	82492	87599	3.31%	0.453%
19	11.108	831	833	835	rBV	43558	39673	1.50%	0.205%
20	11.233	842	844	846	rBV	871729	856728	32.33%	4.426%
21	12.662	966	969	973	rBV	18985	41569	1.57%	0.215%
22	12.811	980	982	985	rBV	1459701	1284697	48.49%	6.637%
23	13.714	1059	1061	1068	rBV	25863	60272	2.27%	0.311%
24	13.862	1071	1074	1076	rBV	573561	681093	25.71%	3.519%
25	14.617	1137	1140	1146	rBV	60447	91170	3.44%	0.471%
26	14.868	1159	1162	1167	rBV	24795	52214	1.97%	0.270%
27	15.200	1189	1191	1193	rBV	20123	26715	1.01%	0.138%
28	15.245	1193	1195	1198	rBV	549093	654152	24.69%	3.380%

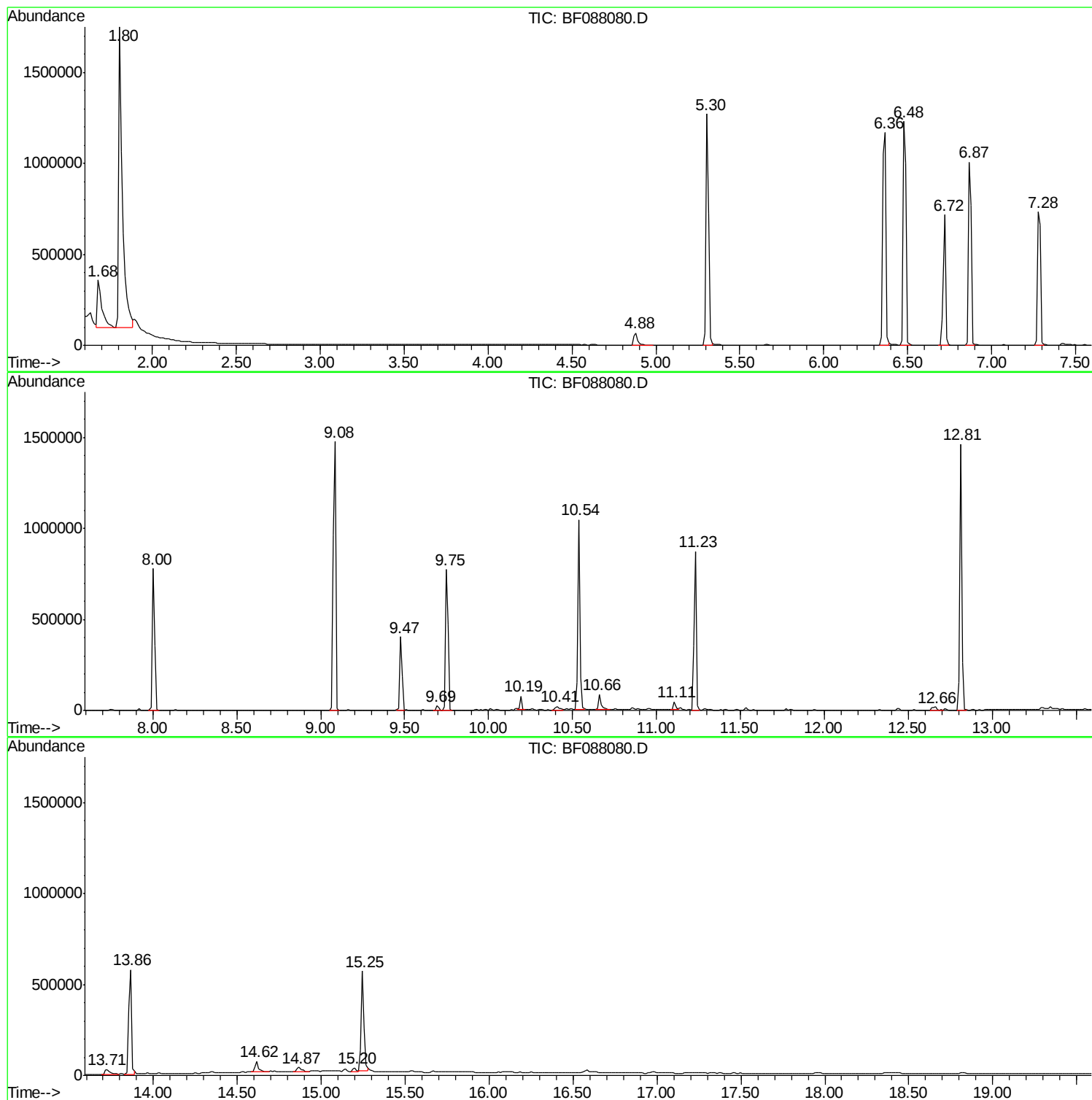
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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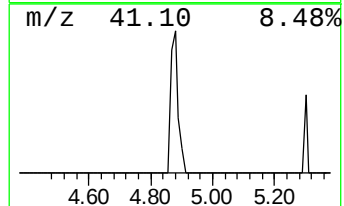
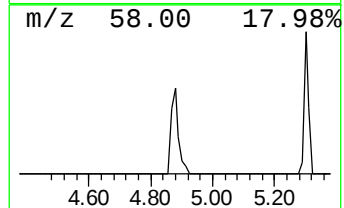
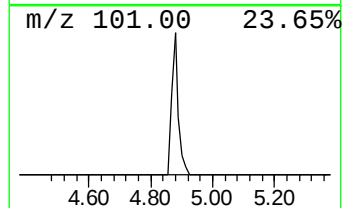
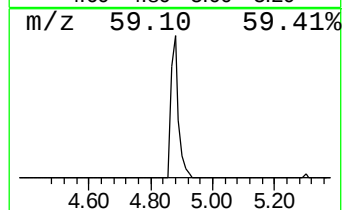
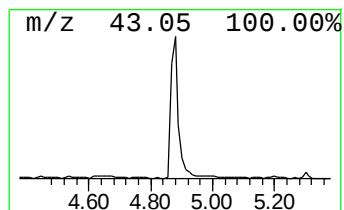
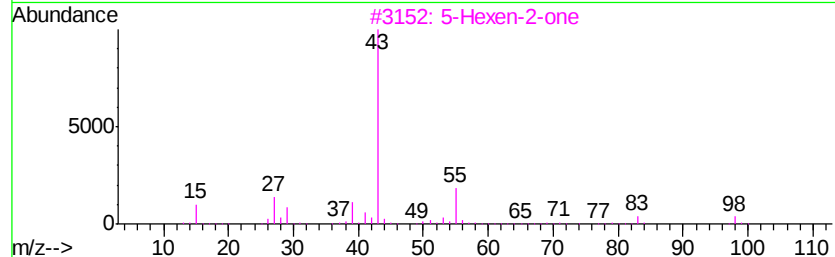
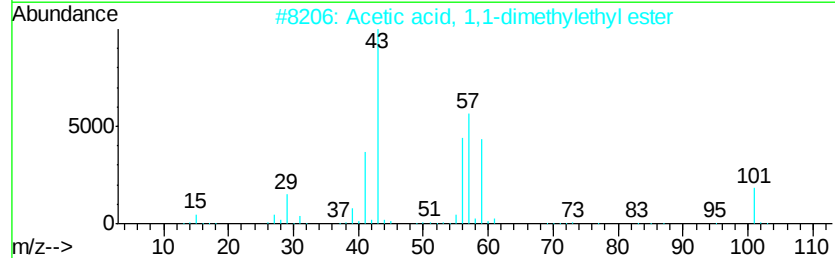
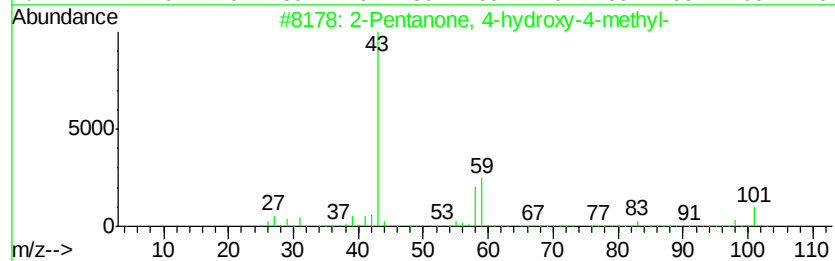
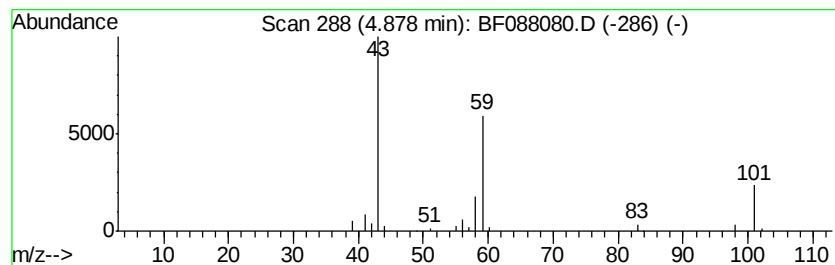
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.88	3.49 ng	107283	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		5-Hexen-2-one	98	C6H10O	000109-49-9	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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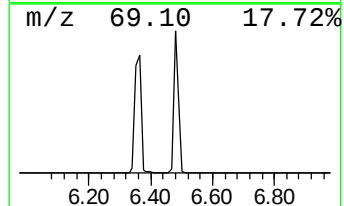
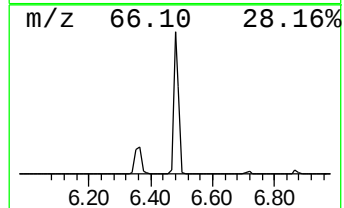
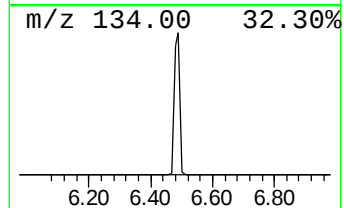
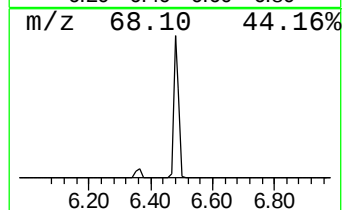
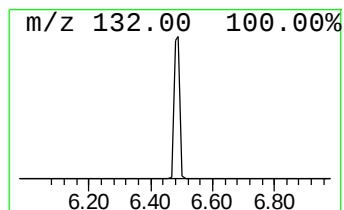
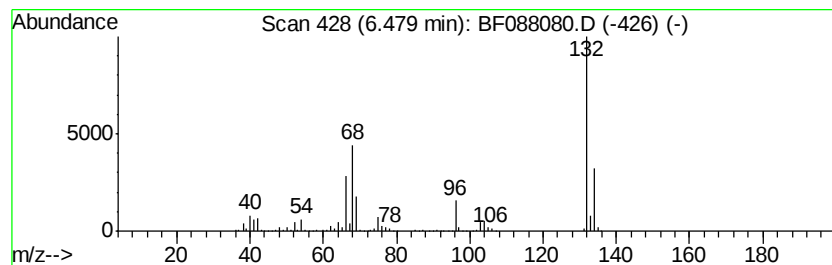
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	50.45 ng	1550970	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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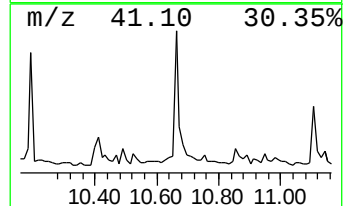
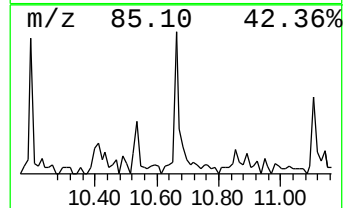
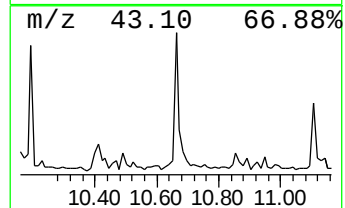
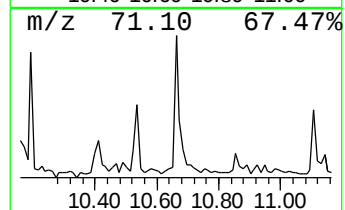
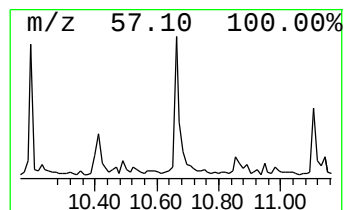
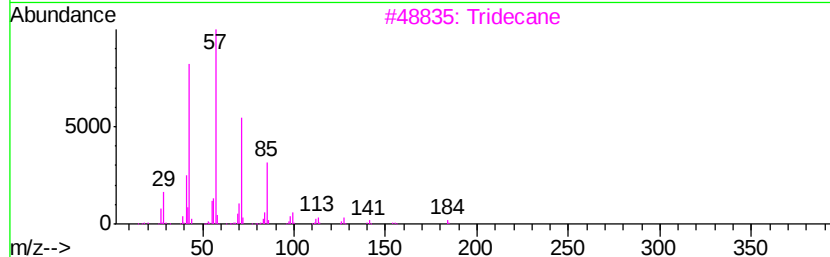
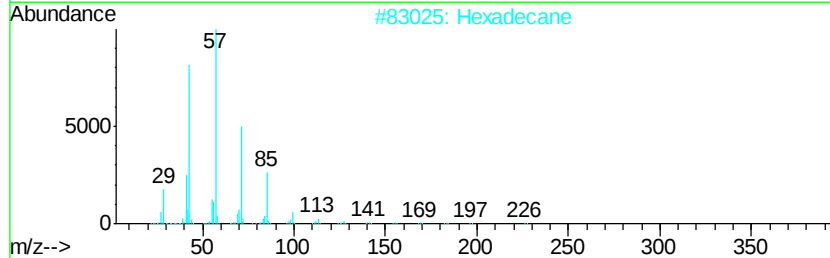
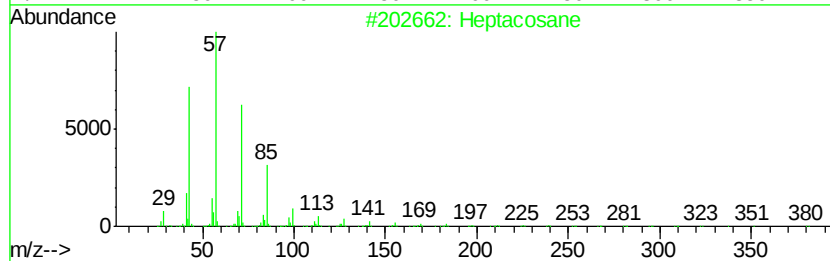
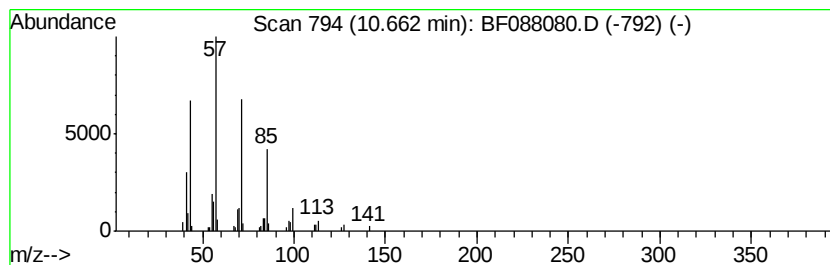
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Peak Number 6 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.66	2.04 ng	87599	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Nonadecane	268	C19H40	000629-92-5	87
5	Heptadecane	240	C17H36	000629-78-7	87



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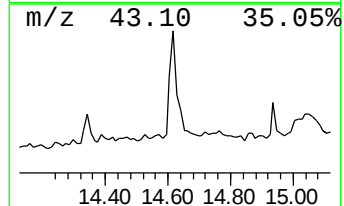
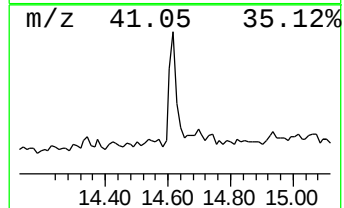
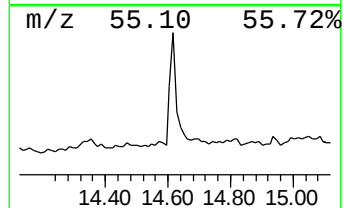
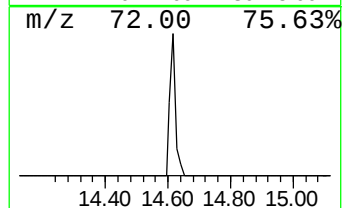
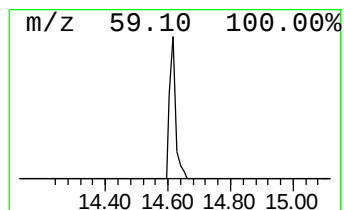
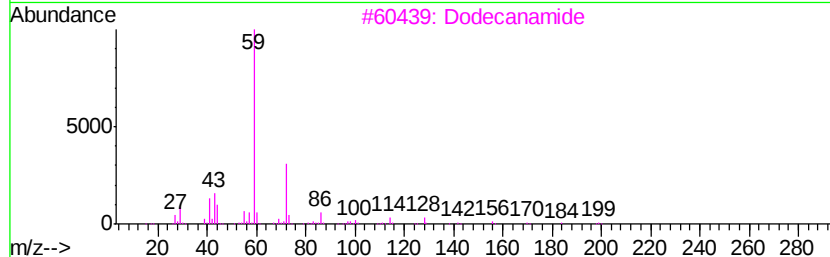
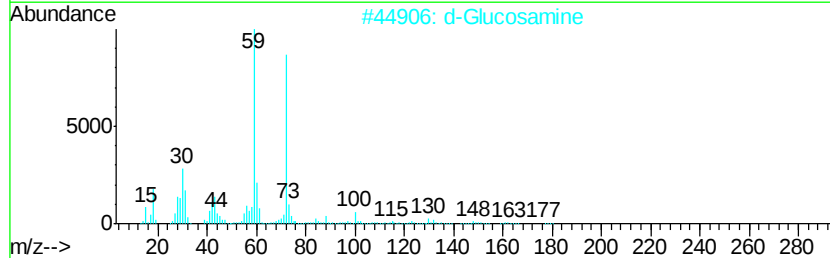
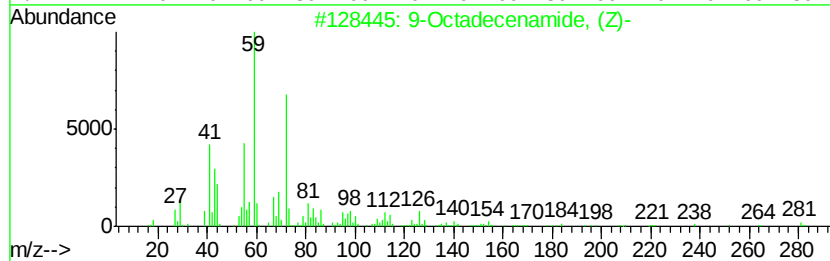
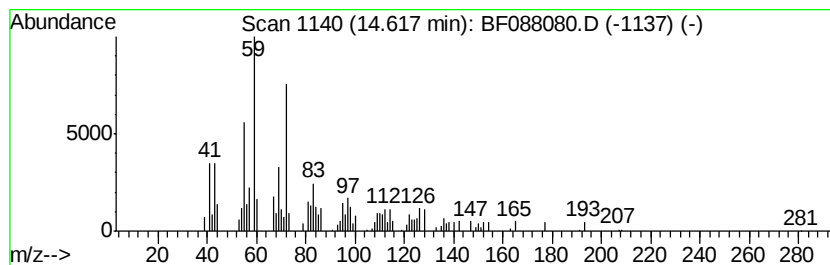
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Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.79 ng	91170	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		d-Glucosamine	179	C6H13NO5	000090-77-7	50
3		Dodecanamide	199	C12H25NO	001120-16-7	47
4		Hexadecanamide	255	C16H33NO	000629-54-9	47
5		1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.88	3.5	ng	107283	1	6.72	614820	20.0
unknown6.48	6.48	50.5	ng	1550970	1	6.72	614820	20.0
Heptacosane	10.66	2.0	ng	87599	4	11.23	856728	20.0
9-Octadecenamide,...	14.62	2.8	ng	91170	6	15.25	654152	20.0