

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061616\
 Data File : BF088082.D
 Acq On : 16 Jun 2016 18:21
 Operator : UM/SJ
 Sample : H3571-09
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-23-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	6	8	17	rVB	215980	441714	12.35%	1.649%
2	1.804	17	19	68	rVB	1618217	3575721	100.00%	13.349%
3	4.890	286	289	295	rBV	82342	144571	4.04%	0.540%
4	5.313	323	326	328	rBV	2054696	2377415	66.49%	8.876%
5	6.365	415	418	420	rBV	1878856	2119132	59.26%	7.911%
6	6.490	426	429	431	rBV	2202517	2440609	68.26%	9.112%
7	6.719	447	449	451	rBV	772096	659301	18.44%	2.461%
8	6.879	460	463	465	rBV	1604824	1966291	54.99%	7.341%
9	7.290	496	499	501	rBV	1559700	1676263	46.88%	6.258%
10	7.919	552	554	556	rBV	62964	54977	1.54%	0.205%
11	7.999	559	561	564	rBV	819797	817353	22.86%	3.051%
12	9.085	653	656	658	rBV	2699328	2683231	75.04%	10.017%
13	9.485	688	691	693	rVB	636622	843918	23.60%	3.151%
14	9.748	712	714	717	rBB	742240	907784	25.39%	3.389%
15	10.536	781	783	786	rBV2	1221708	1428024	39.94%	5.331%
16	11.234	842	844	846	rBV	974937	921404	25.77%	3.440%
17	12.651	966	968	971	rBV2	86632	126887	3.55%	0.474%
18	12.811	980	982	985	rBV	1596973	2046428	57.23%	7.640%
19	13.348	1027	1029	1031	rBV	62455	52067	1.46%	0.194%
20	13.725	1060	1062	1066	rBV	27145	42708	1.19%	0.159%
21	13.862	1071	1074	1076	rBV	664171	707276	19.78%	2.640%
22	14.617	1137	1140	1145	rBV2	60918	99232	2.78%	0.370%
23	15.245	1193	1195	1198	rBV	531799	653606	18.28%	2.440%

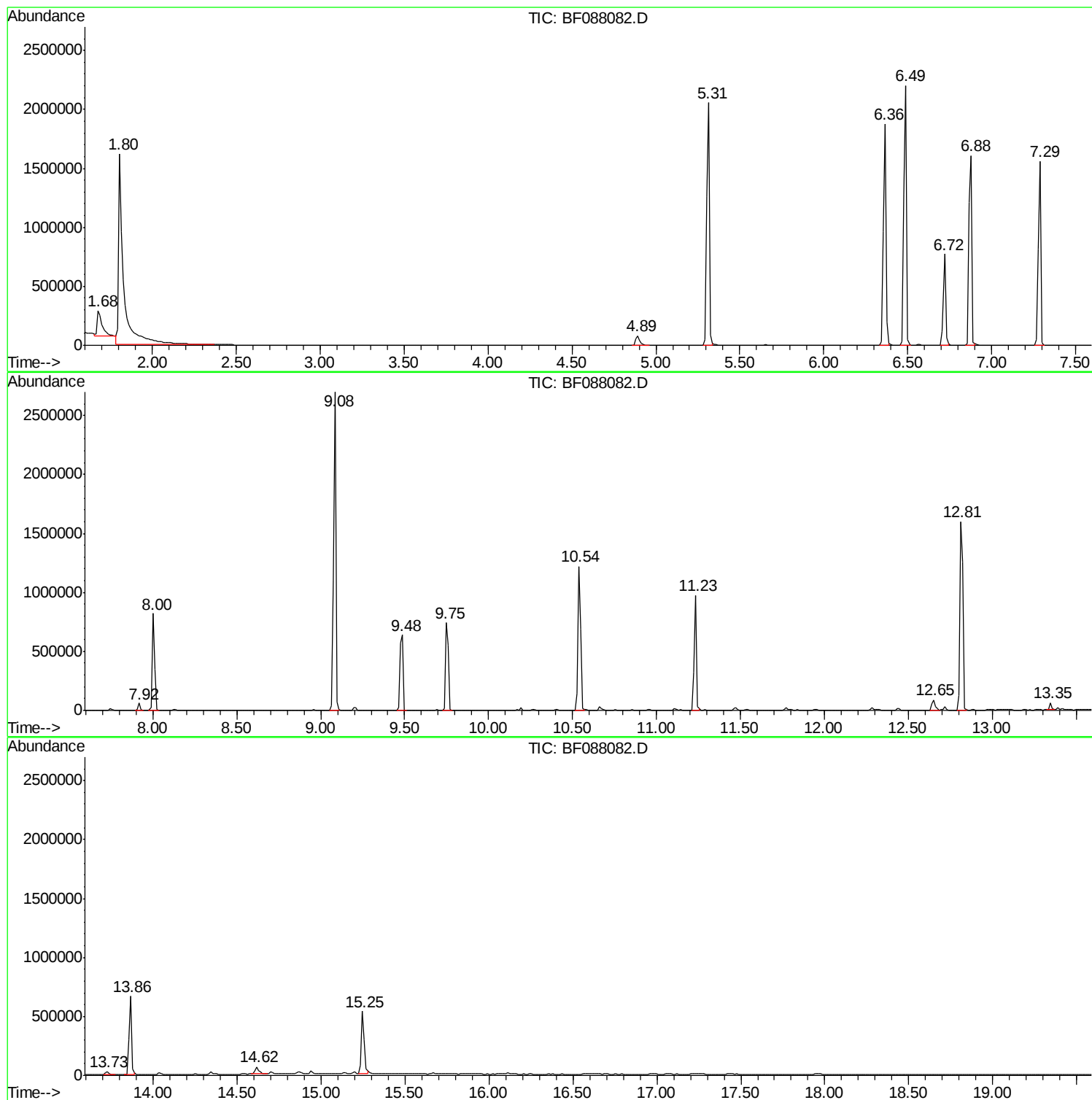
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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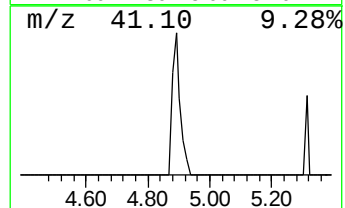
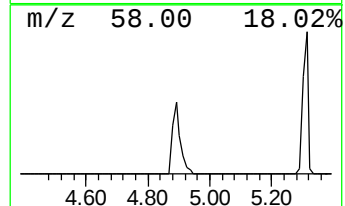
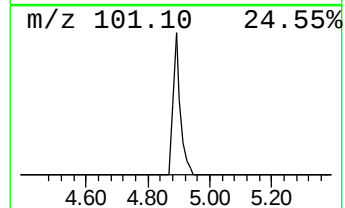
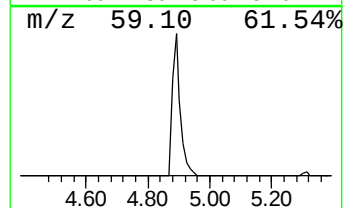
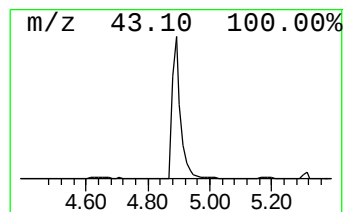
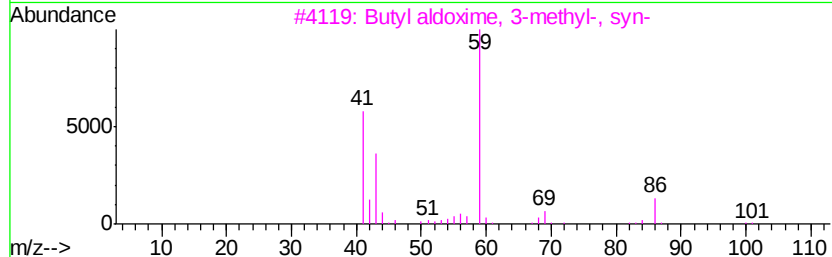
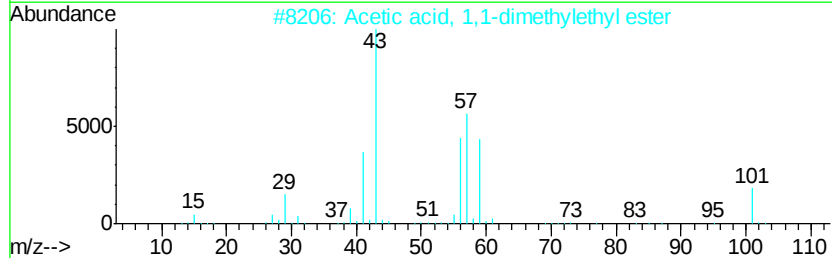
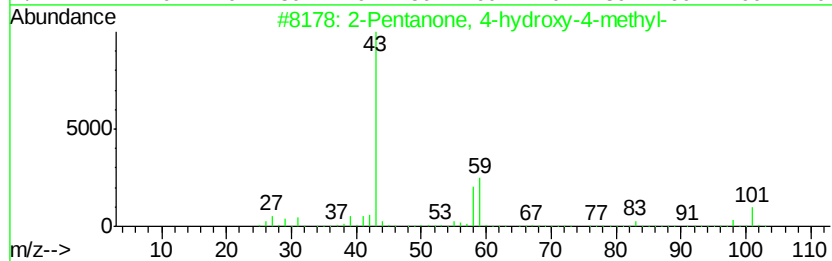
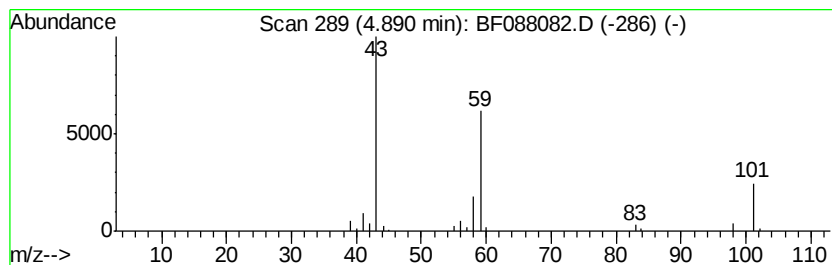
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.89	4.39 ng	144571	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	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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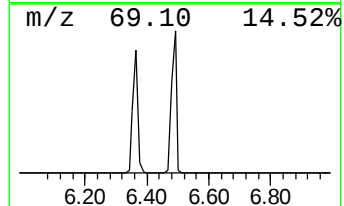
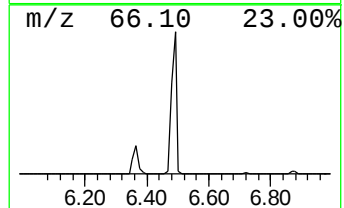
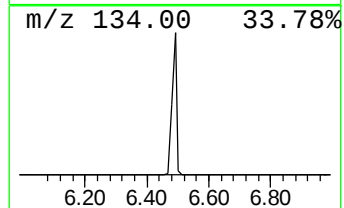
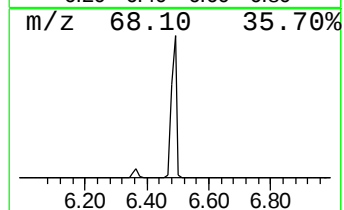
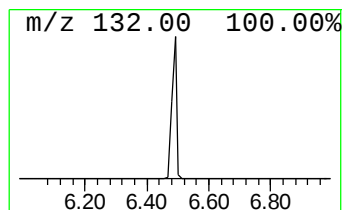
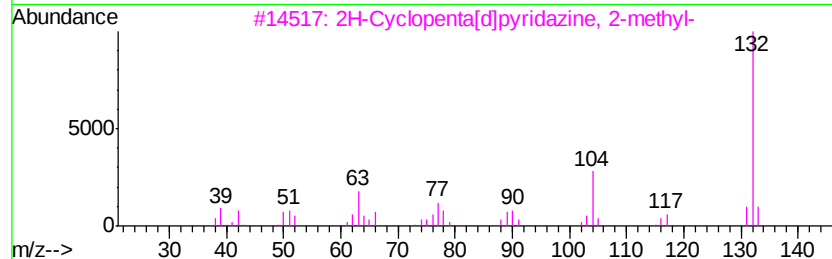
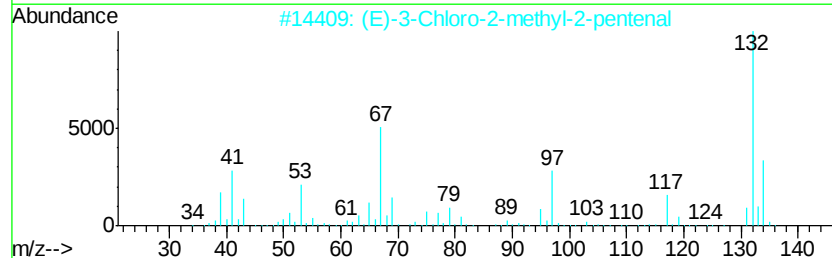
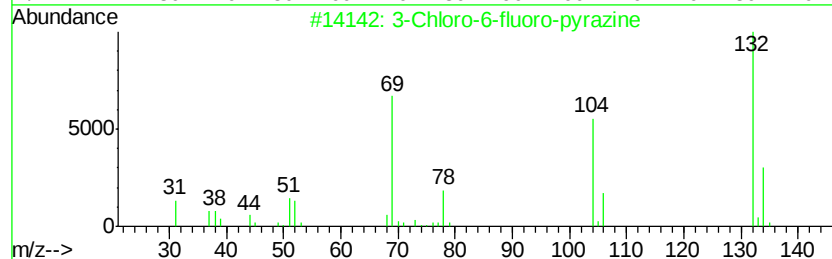
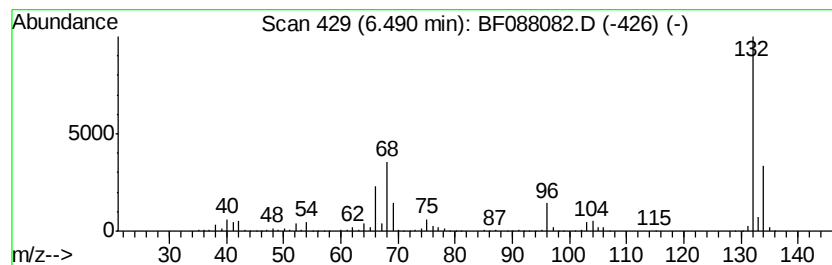
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Peak Number 4 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	74.04 ng	2440610	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		2H-Cyclopentaf[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



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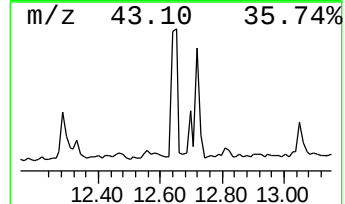
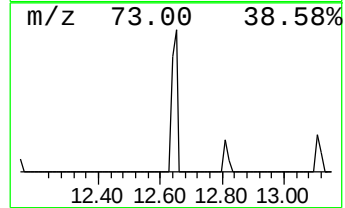
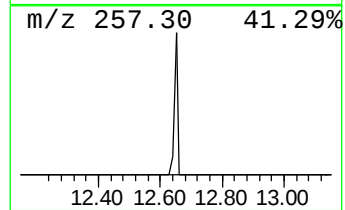
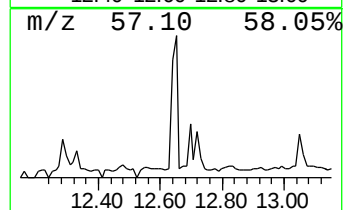
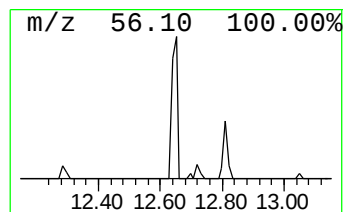
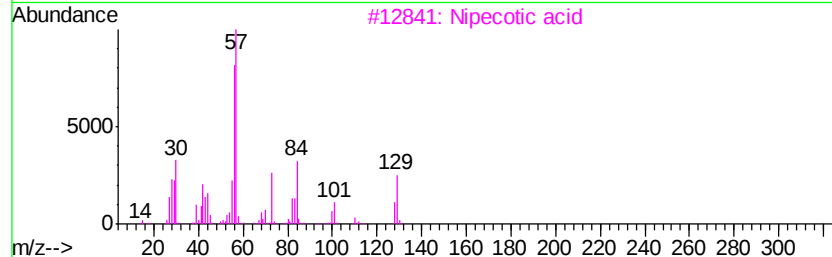
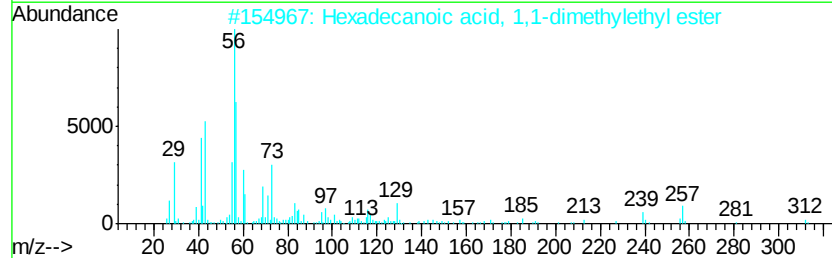
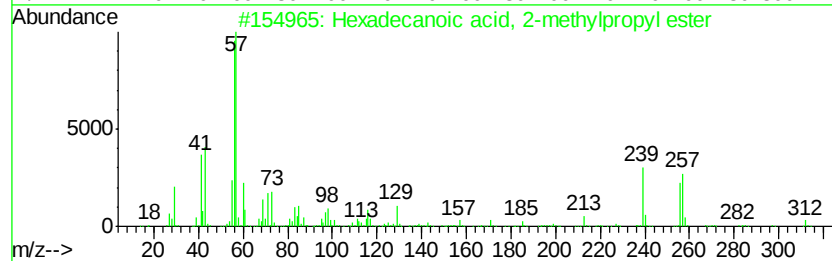
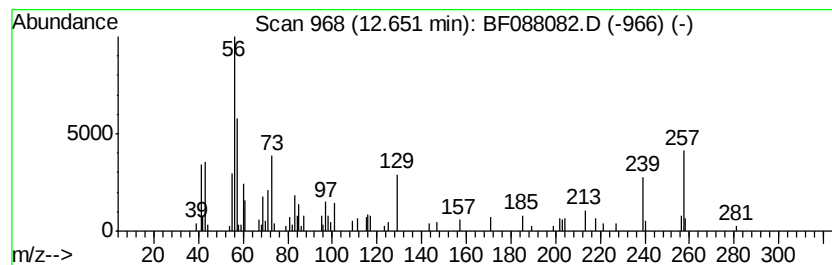
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Peak Number 6 Hexadecanoic acid, 2-methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	3.59 ng	126887	Chrysene-d12	13.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	72
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
3			Nipecotic acid	129	C6H11NO2	000498-95-3	32
4			Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	27
5			Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	25



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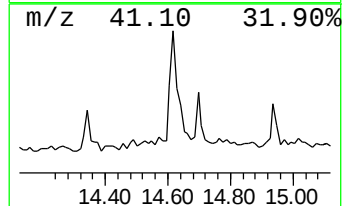
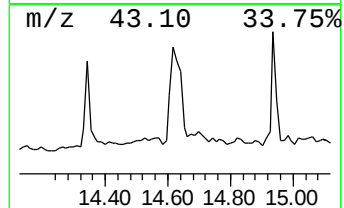
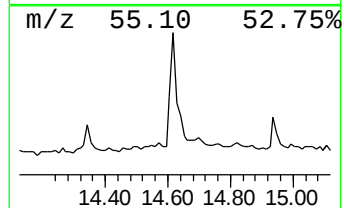
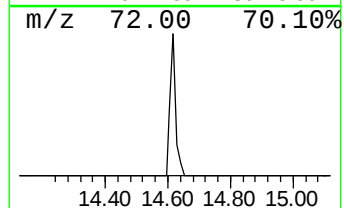
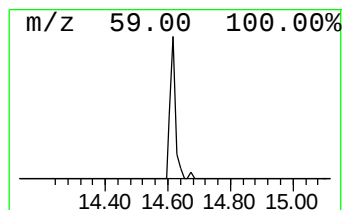
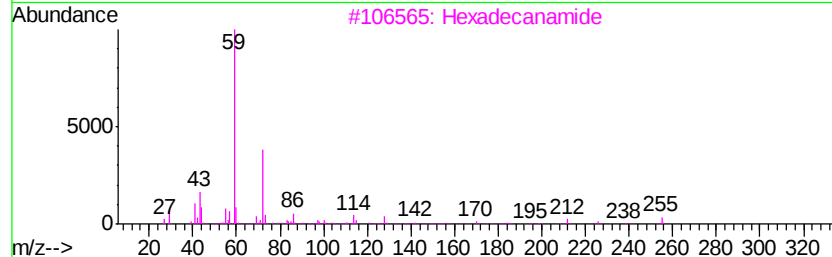
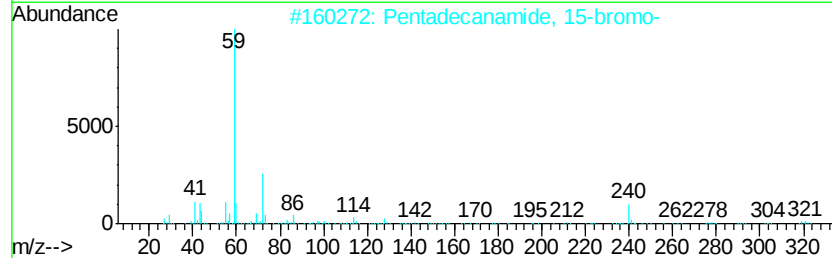
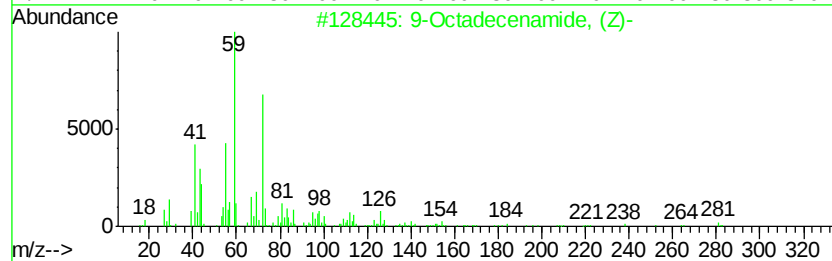
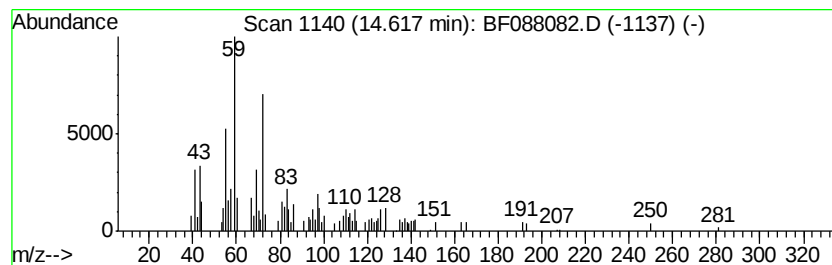
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Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.04 ng	99232	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
3		Hexadecanamide	255	C16H33NO	000629-54-9	59
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Tetradecanamide	227	C14H29NO	000638-58-4	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	4.4	ng	144571	1	6.72	659301	20.0
unknown6.49	6.49	74.0	ng	2440610	1	6.72	659301	20.0
Hexadecanoic acid...	12.65	3.6	ng	126887	5	13.86	707276	20.0
9-Octadecenamide,...	14.62	3.0	ng	99232	6	15.25	653606	20.0