

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061416\
 Data File : BF088027.D
 Acq On : 15 Jun 2016 5:18
 Operator : UM/SJ
 Sample : H3425-05
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP16-LF2MW2

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	1.724	11	12	21	rVB	189937	295861	8.14%	1.366%
2	1.850	21	23	76	rVB	1685498	3633660	100.00%	16.781%
3	4.936	291	293	298	rBV	82006	92327	2.54%	0.426%
4	5.370	329	331	334	rBV	1279467	1161805	31.97%	5.366%
5	6.410	420	422	425	rBV	599558	703760	19.37%	3.250%
6	6.547	432	434	437	rBV	1991376	1903618	52.39%	8.792%
7	6.776	452	454	457	rBV	504242	570915	15.71%	2.637%
8	6.936	466	468	471	rVB	1889598	1850875	50.94%	8.548%
9	7.347	501	504	507	rBV	1344571	1458484	40.14%	6.736%
10	8.067	565	567	569	rBV	938675	764963	21.05%	3.533%
11	9.153	659	662	664	rBV	2776396	2851214	78.47%	13.168%
12	9.828	718	721	723	rBB	590353	715362	19.69%	3.304%
13	10.605	787	789	792	rBV2	853107	1224602	33.70%	5.656%
14	11.302	848	850	853	rBV	748449	611346	16.82%	2.823%
15	12.719	972	974	976	rBB	205502	165610	4.56%	0.765%
16	12.799	976	981	983	rBB2	36478	43677	1.20%	0.202%
17	12.891	986	989	992	rBV	2102670	2024689	55.72%	9.351%
18	13.428	1033	1036	1038	rBV	114217	123158	3.39%	0.569%
19	13.474	1038	1040	1043	rVV	20883	39997	1.10%	0.185%
20	13.931	1078	1080	1083	rBV2	533849	633700	17.44%	2.927%
21	14.114	1093	1096	1098	rBV	41944	36826	1.01%	0.170%
22	14.422	1120	1123	1125	rBV	26151	36429	1.00%	0.168%
23	14.708	1146	1148	1151	rBV	37088	42882	1.18%	0.198%
24	15.028	1173	1176	1178	rBV	44285	44624	1.23%	0.206%
25	15.348	1201	1204	1206	rBV	343025	500915	13.79%	2.313%
26	15.382	1206	1207	1210	rVB	41279	38836	1.07%	0.179%
27	15.782	1239	1242	1247	rVB	29359	44402	1.22%	0.205%
28	16.251	1279	1283	1286	rVB2	20932	38301	1.05%	0.177%

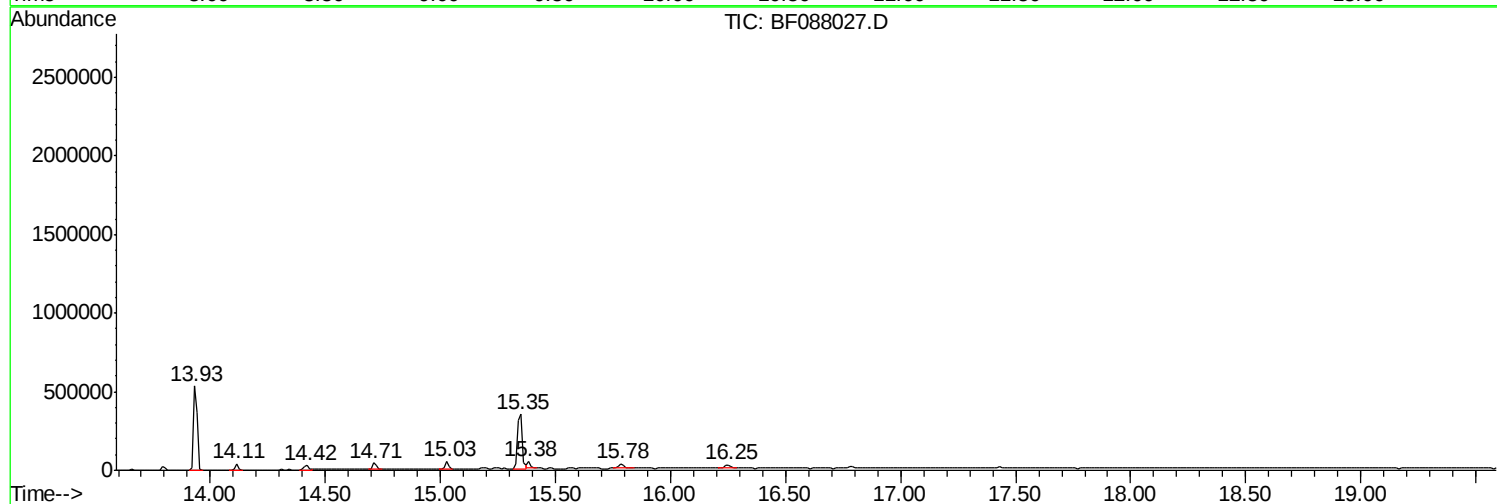
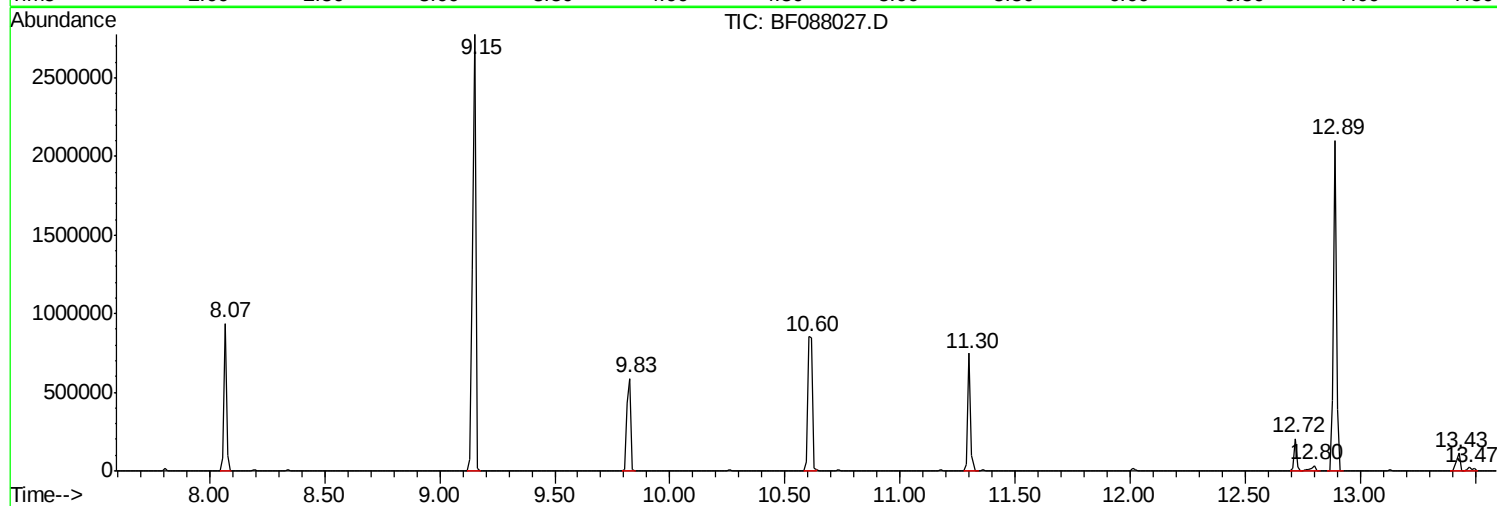
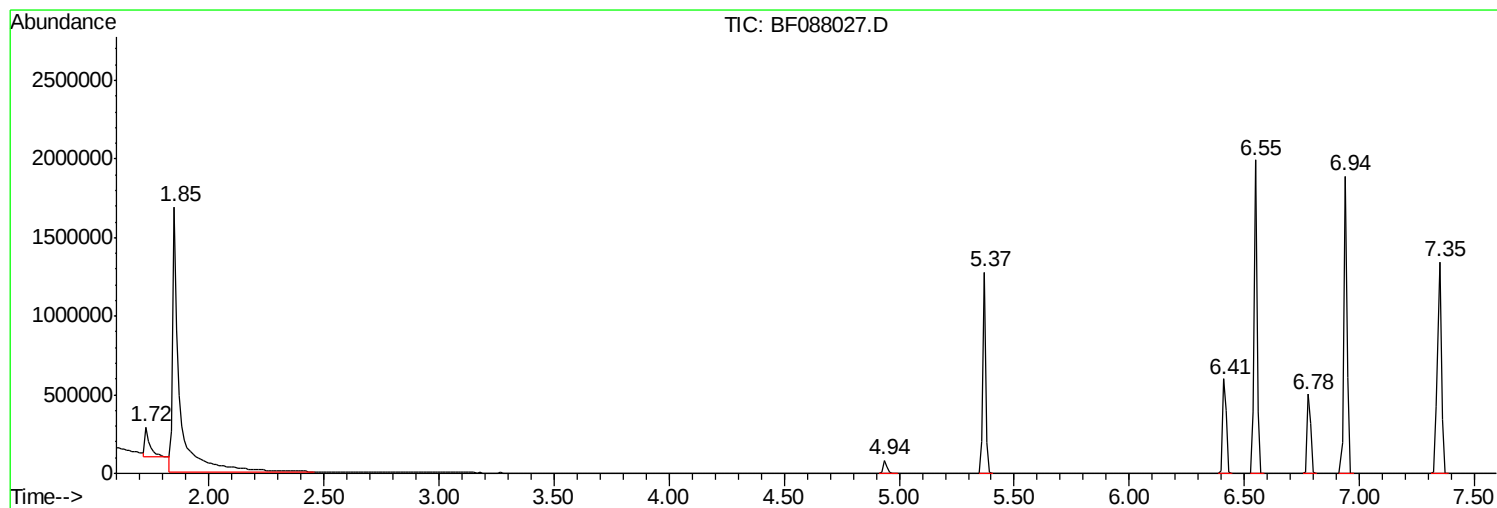
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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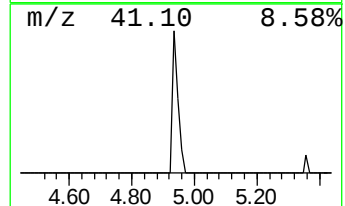
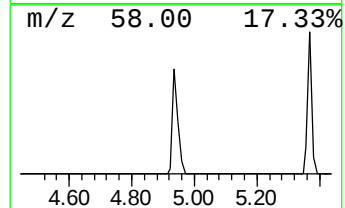
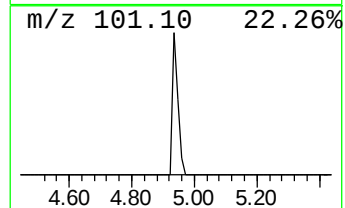
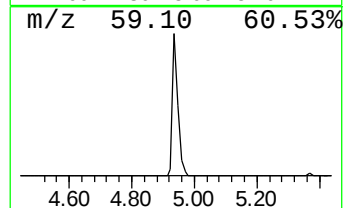
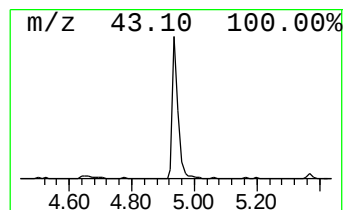
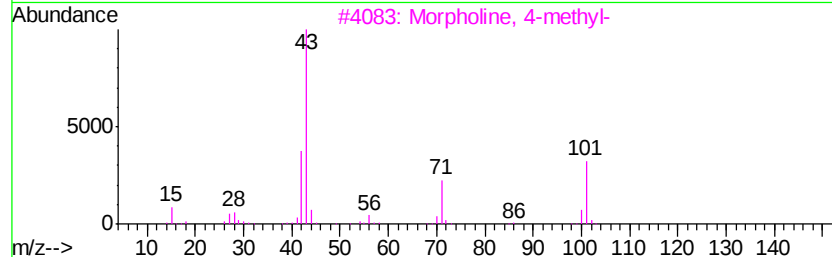
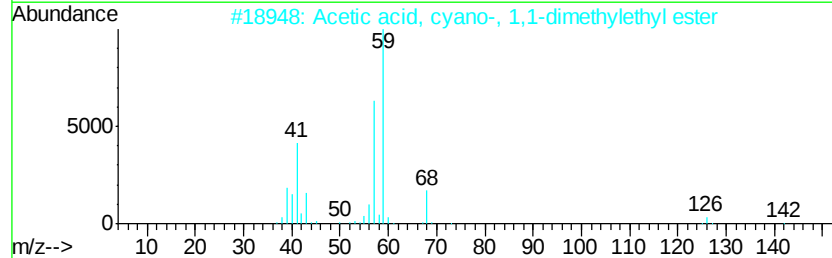
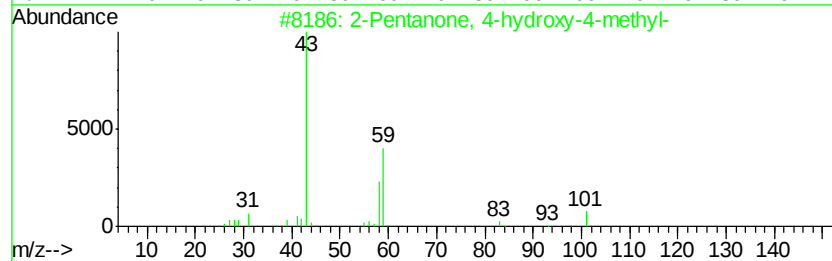
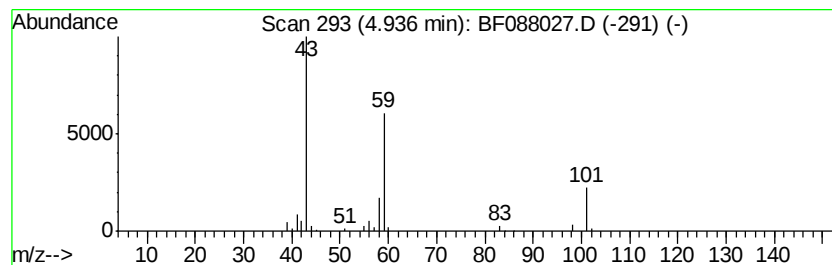
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	3.23 ng	92327	1,4-Dichlorobenzene-d4	6.78

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	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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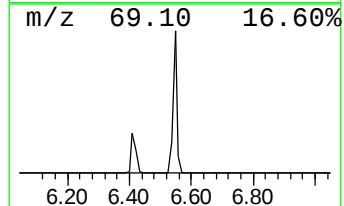
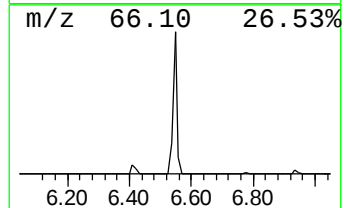
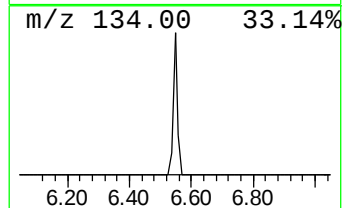
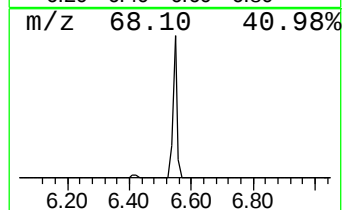
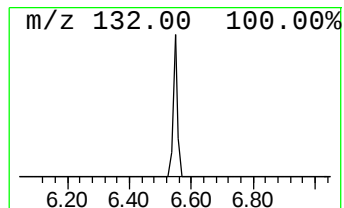
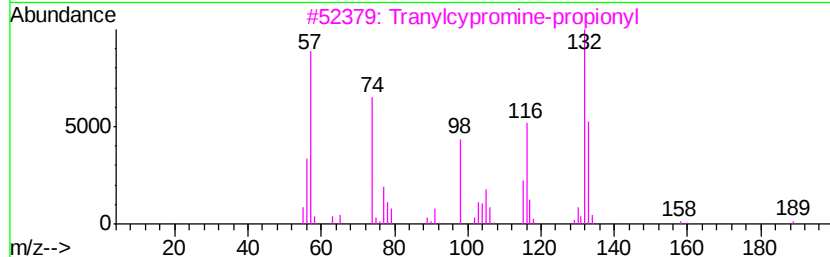
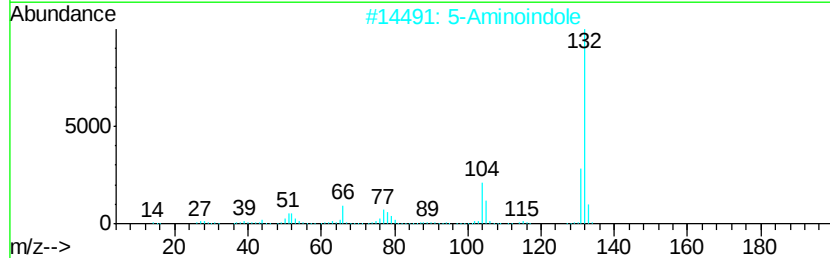
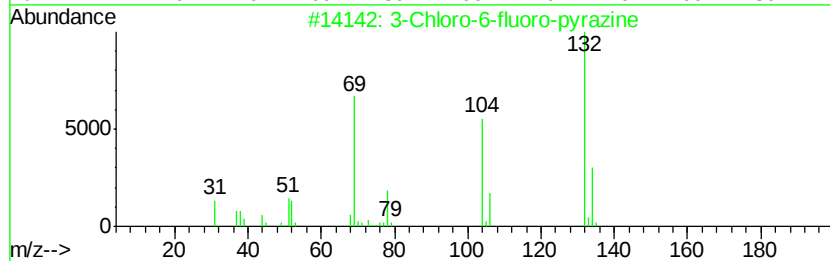
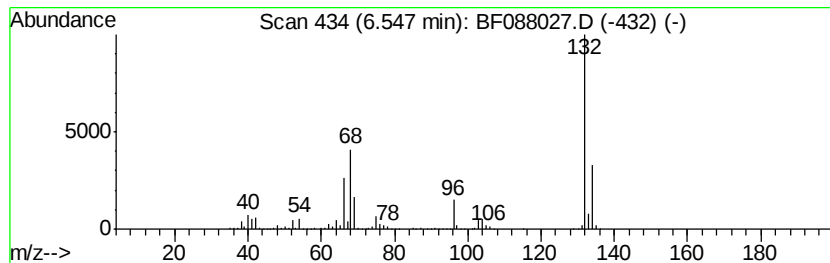
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Peak Number 4 unknown6.55 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	66.69 ng	1903620	1,4-Dichlorobenzene-d4	6.78

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			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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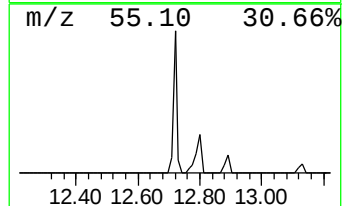
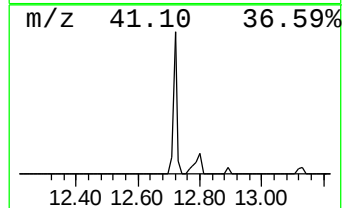
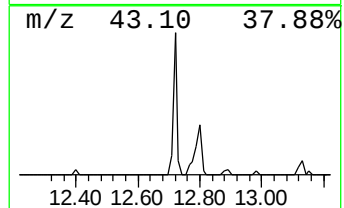
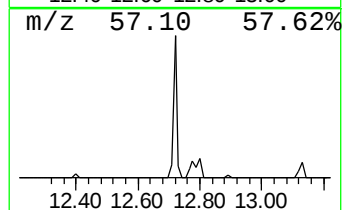
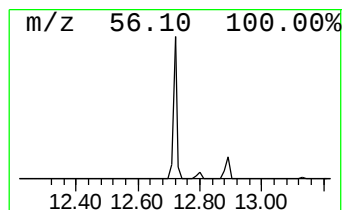
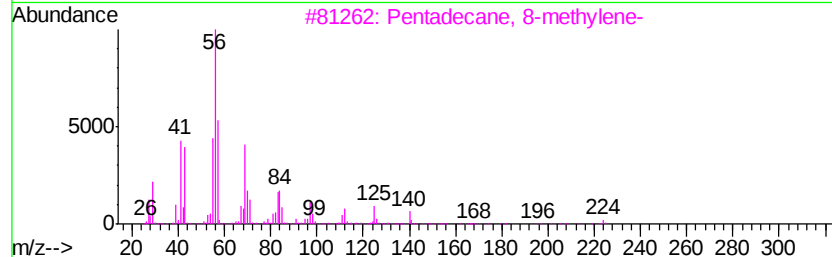
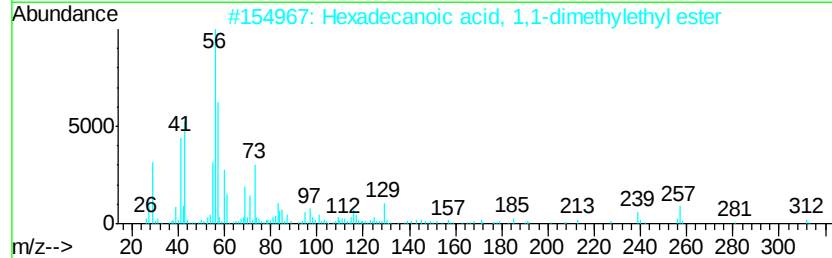
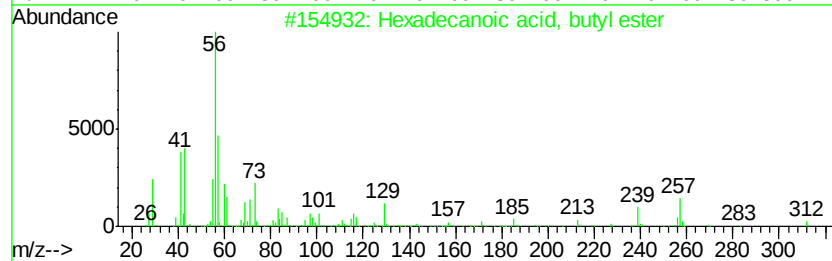
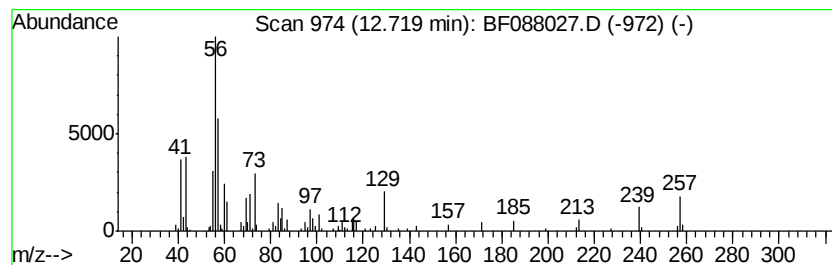
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	5.23 ng	165610	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5		2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27



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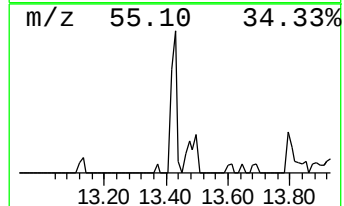
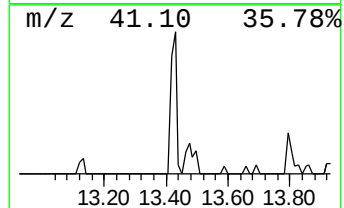
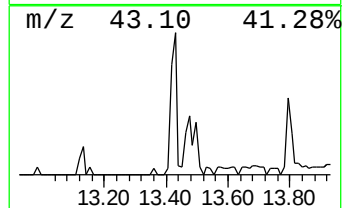
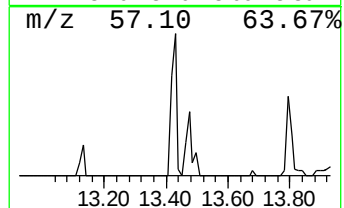
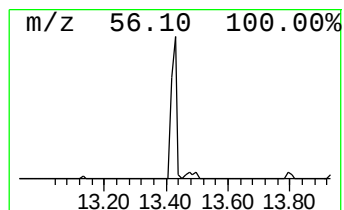
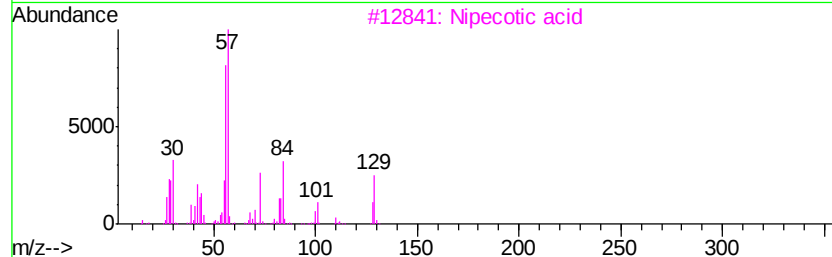
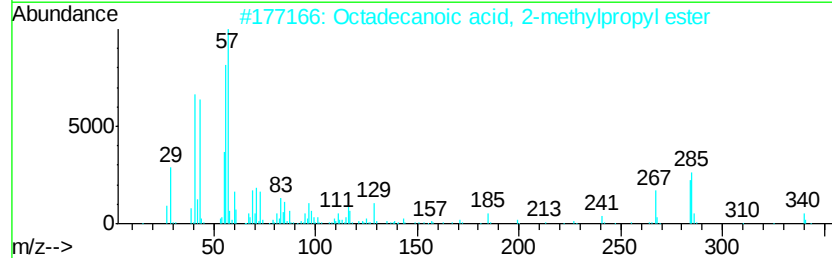
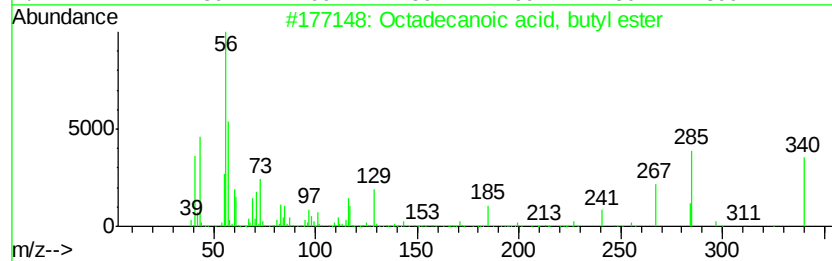
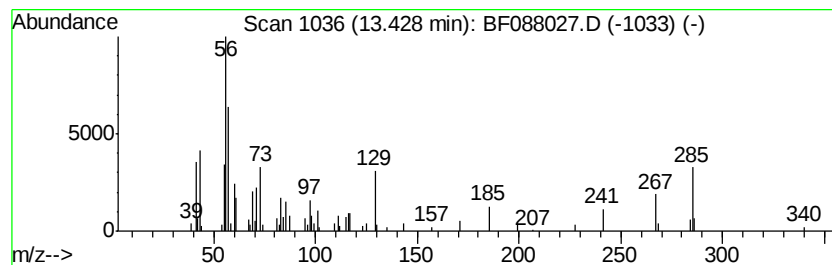
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Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	3.89 ng	123158	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	80
3		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	32
5		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.94	3.2	ng	92327	1	6.78	570915	20.0
unknown6.55	6.55	66.7	ng	1903620	1	6.78	570915	20.0
Hexadecanoic acid...	12.72	5.2	ng	165610	5	13.93	633700	20.0
Octadecanoic acid...	13.43	3.9	ng	123158	5	13.93	633700	20.0