

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100217\
 Data File : BF099000.D
 Acq On : 2 Oct 2017 15:32
 Operator : SJ/JU
 Sample : PB102839BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB102839BL

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-BF092317.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	5.145	515	520	532	rBV	430269	597345	15.27%	1.978%
2	5.534	580	586	589	rBV	3134308	3286081	83.99%	10.880%
3	6.528	749	755	758	rBV	2897544	3238065	82.77%	10.721%
4	6.675	775	780	783	rBV	3174022	3362015	85.93%	11.131%
5	6.898	815	818	822	rBV	860771	744133	19.02%	2.464%
6	7.057	841	845	848	rBV	2859890	2698341	68.97%	8.934%
7	7.463	908	914	917	rBV	1995979	2140042	54.70%	7.085%
8	8.181	1031	1036	1040	rBV	1051759	1013538	25.91%	3.356%
9	9.257	1213	1219	1222	rBV	3497098	3912301	100.00%	12.953%
10	9.939	1330	1335	1339	rBV2	1183584	1101027	28.14%	3.645%
11	10.727	1463	1469	1473	rBV	1807236	1978504	50.57%	6.551%
12	11.427	1583	1588	1591	rBV	1296157	1058240	27.05%	3.504%
13	12.821	1821	1825	1828	rBV	165785	125823	3.22%	0.417%
14	13.016	1853	1858	1861	rBV	3336438	3319891	84.86%	10.992%
15	13.527	1941	1945	1948	rBV	108683	84810	2.17%	0.281%
16	14.068	2033	2037	2040	rBV	933510	846334	21.63%	2.802%
17	15.557	2284	2290	2298	rBV	545748	697281	17.82%	2.309%

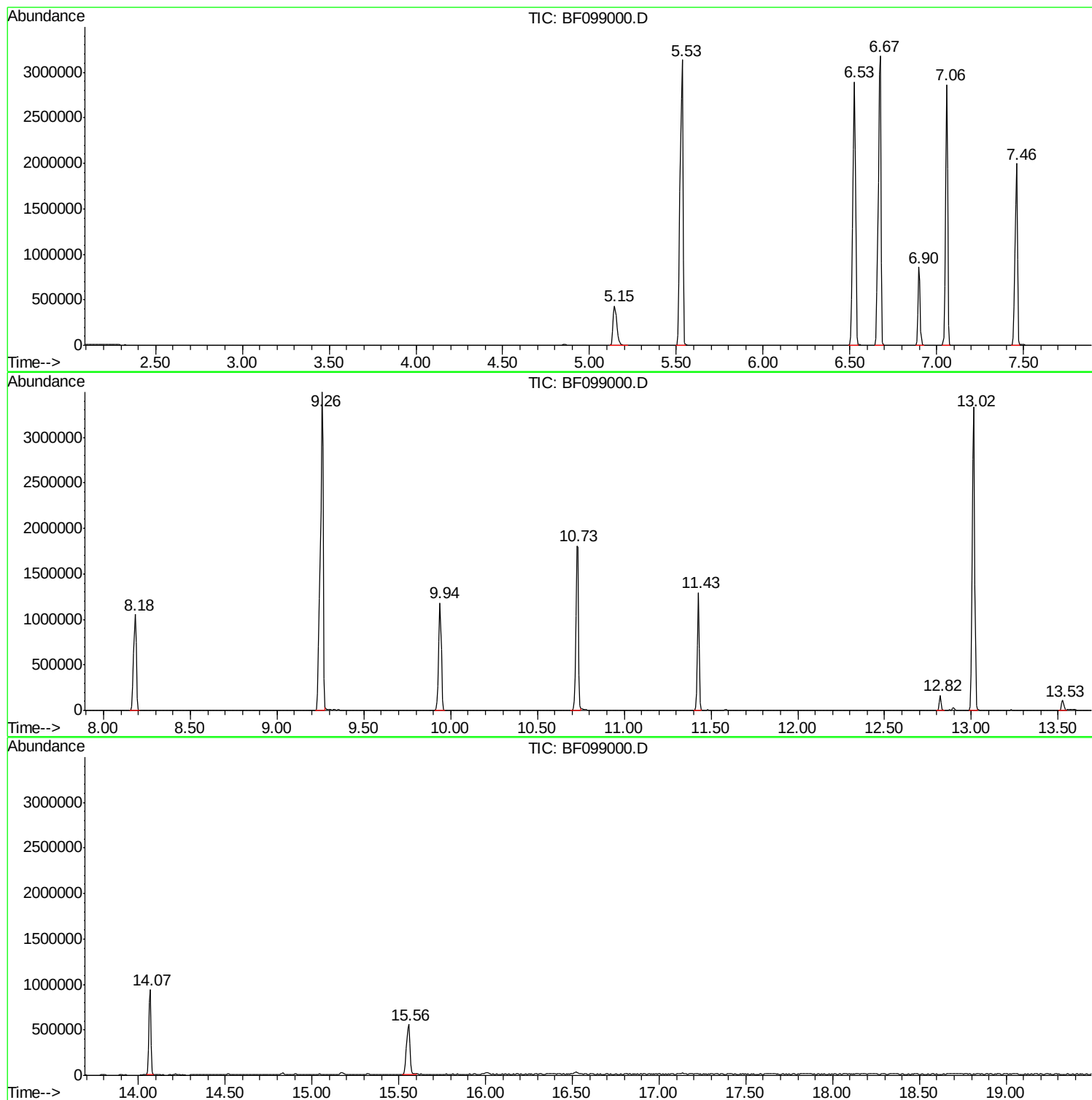
Sum of corrected areas: 30203771

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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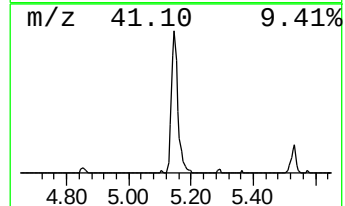
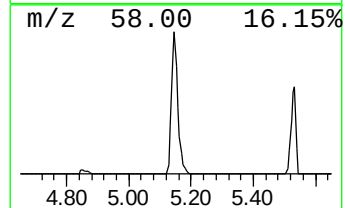
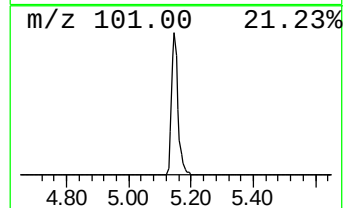
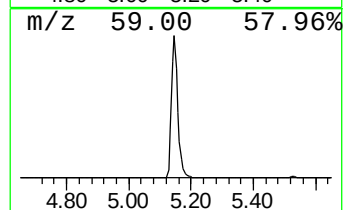
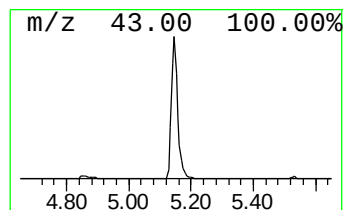
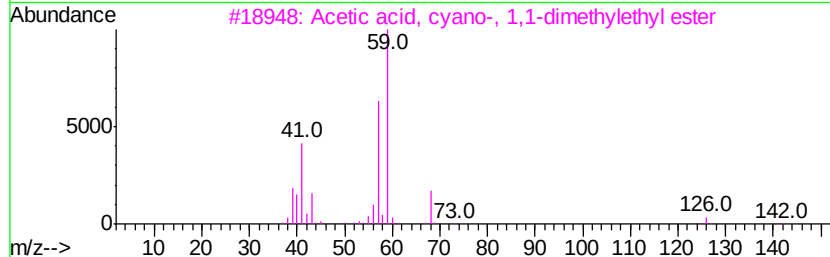
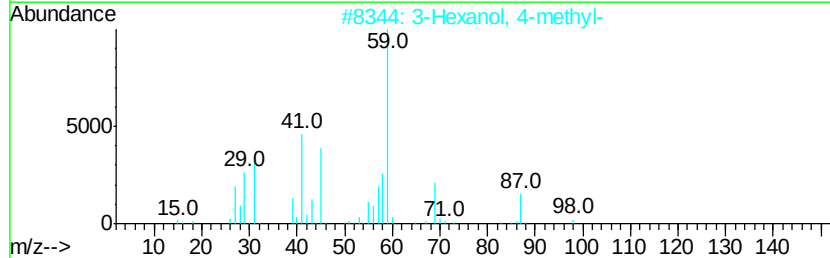
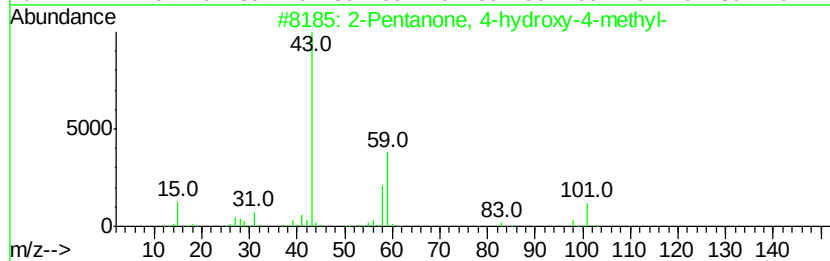
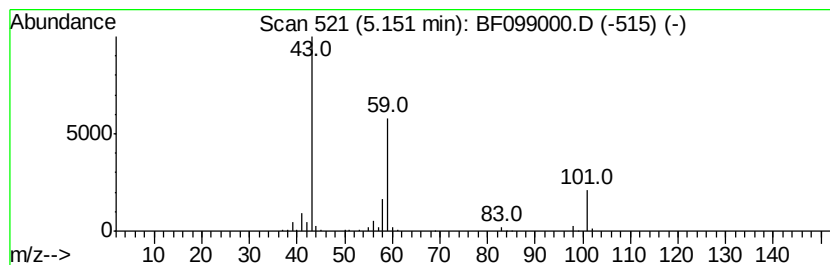
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	16.05 ng	597345	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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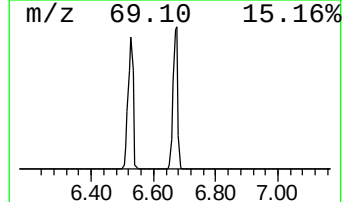
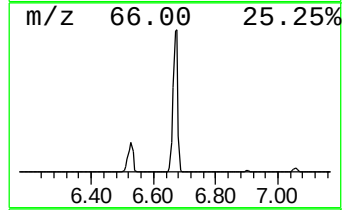
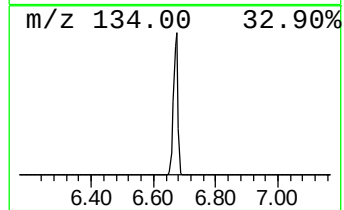
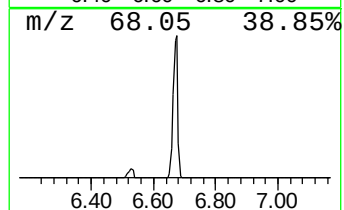
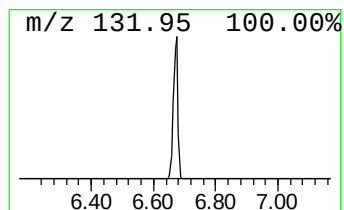
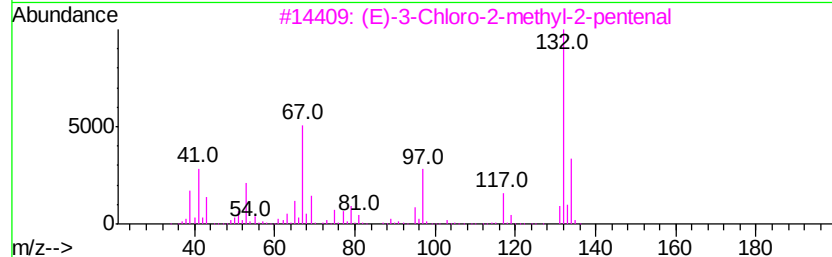
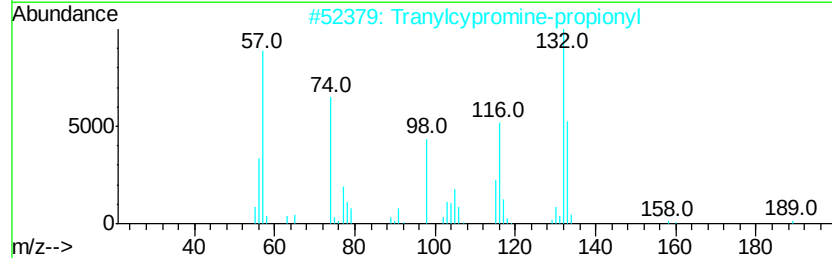
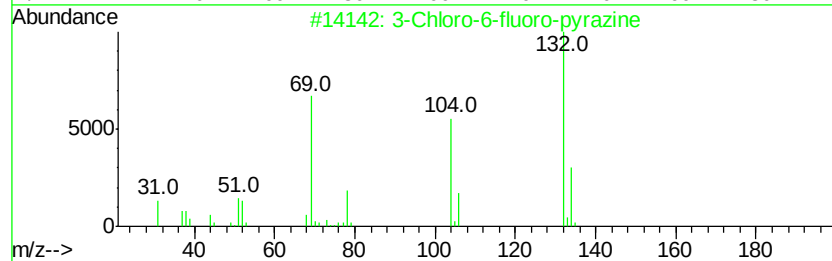
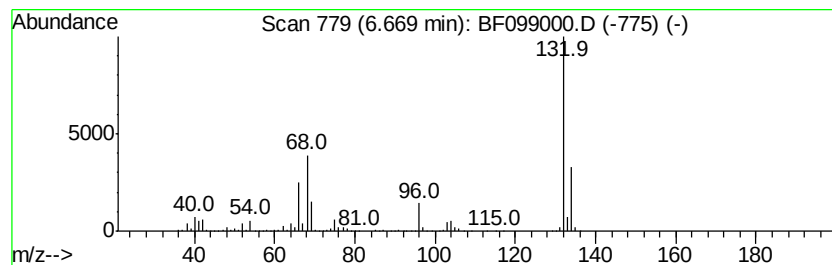
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Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	90.36 ng	3362020	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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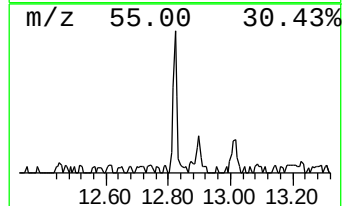
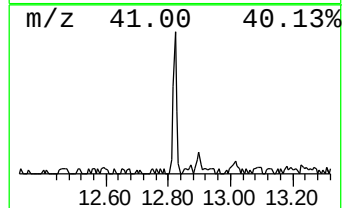
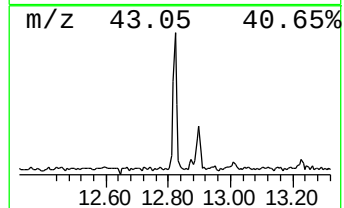
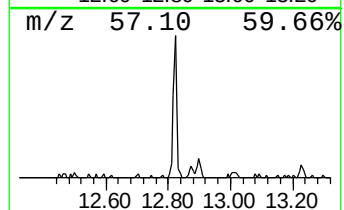
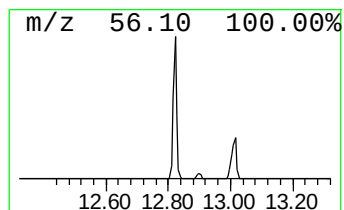
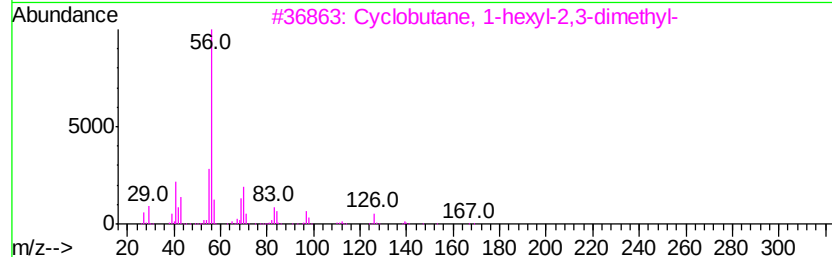
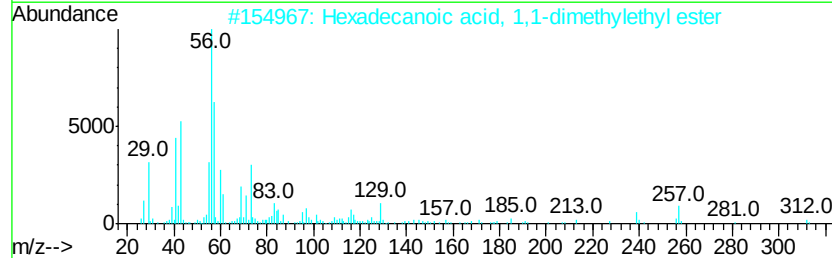
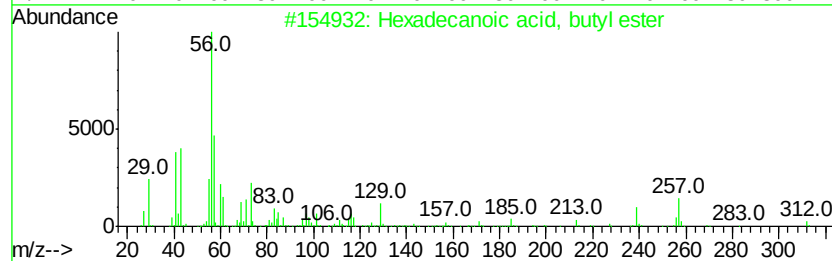
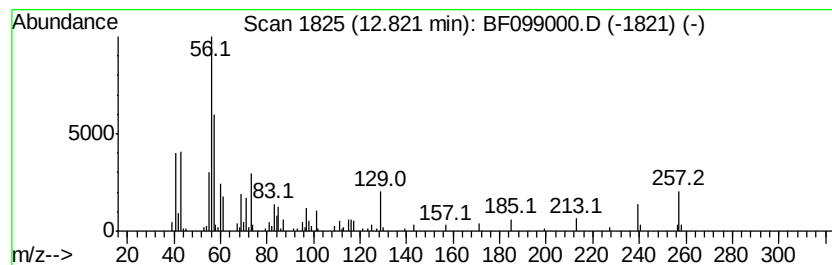
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	2.97 ng	125823	Chrysene-d12	14.07

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	72
3		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27
4		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	27
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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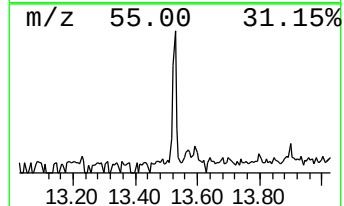
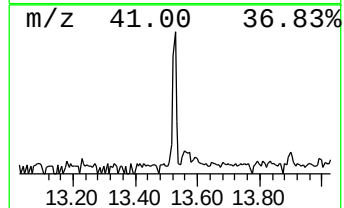
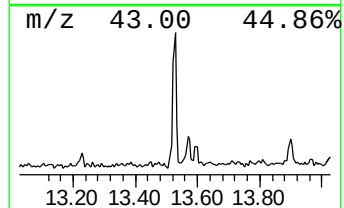
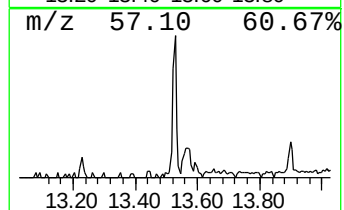
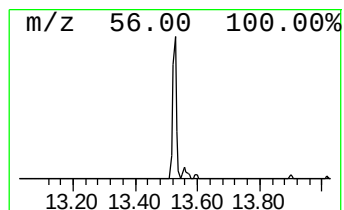
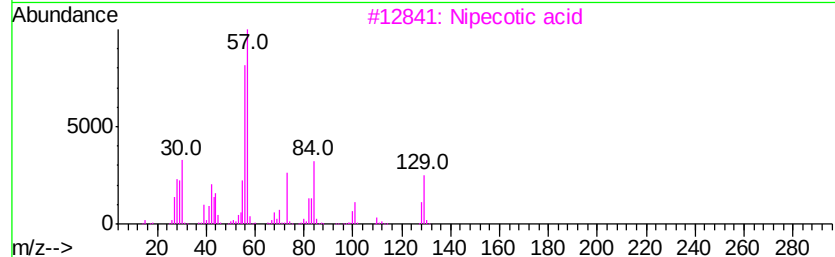
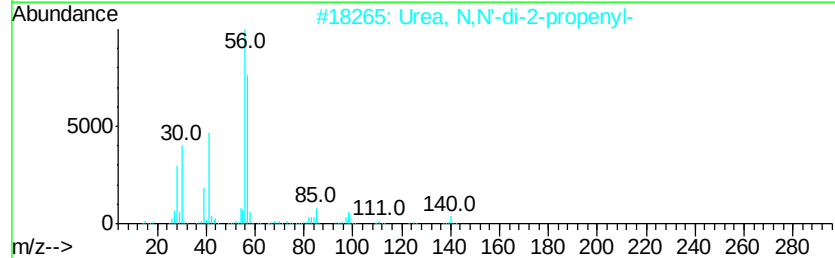
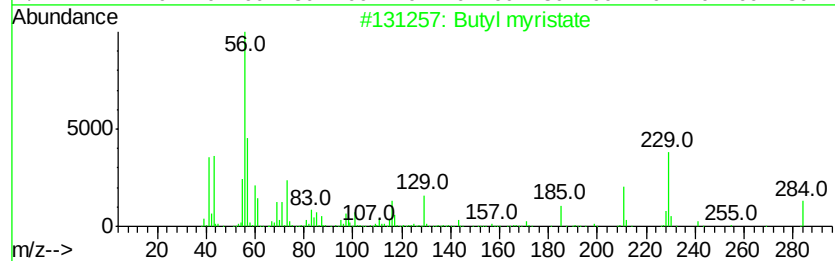
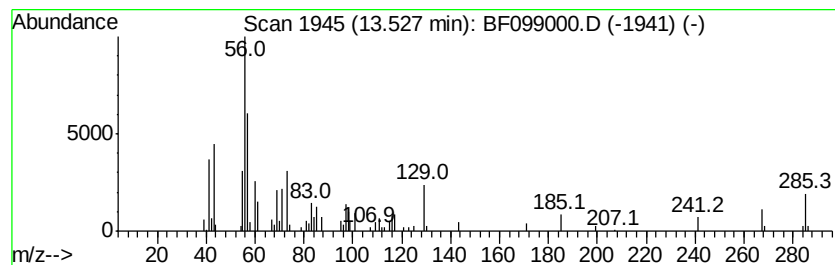
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Peak Number 5 Butyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.53	2.00 ng	84810	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	80
2	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
3	Nipecotic acid	129	C6H11NO2	000498-95-3	37
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	16.1	ng	597345	1	6.90	744133	20.0
unknown6.67	6.67	90.4	ng	3362020	1	6.90	744133	20.0
Hexadecanoic acid...	12.82	3.0	ng	125823	5	14.07	846334	20.0
Butyl myristate	13.53	2.0	ng	84810	5	14.07	846334	20.0