

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012615\
 Data File : BF077051.D
 Acq On : 26 Jan 2015 13:28
 Operator : TP/IZ
 Sample : PB81263BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB81263BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.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	1.327	20	21	26	rBV	20424	35482	3.66%	0.500%
2	1.407	26	28	39	rVB	29396	66168	6.83%	0.932%
3	3.830	238	240	251	rBV	66277	182870	18.89%	2.576%
4	4.790	321	324	336	rBV	363020	687902	71.04%	9.692%
5	7.167	529	532	536	rBV	414485	639512	66.05%	9.010%
6	7.247	536	539	544	rVB	418595	729982	75.39%	10.285%
7	7.762	581	584	589	rBB	93080	145605	15.04%	2.051%
8	8.082	609	612	616	rBV	345298	539348	55.70%	7.599%
9	9.065	694	698	701	rBV	278913	412687	42.62%	5.814%
10	10.676	835	839	842	rBV	119720	203538	21.02%	2.868%
11	13.328	1067	1071	1074	rBV	531555	826463	85.35%	11.644%
12	14.802	1196	1200	1203	rBV	125756	219541	22.67%	3.093%
13	16.517	1347	1350	1353	rBV	356292	489231	50.53%	6.893%
14	17.626	1445	1447	1450	rBV	186346	238129	24.59%	3.355%
15	19.786	1633	1636	1638	rBB	96598	124988	12.91%	1.761%
16	19.877	1641	1644	1646	rBV	872327	968291	100.00%	13.642%
17	20.677	1712	1714	1716	rBB	85714	85577	8.84%	1.206%
18	20.803	1723	1725	1727	rBV	12930	15044	1.55%	0.212%
19	21.134	1752	1754	1757	rBV	231658	248271	25.64%	3.498%
20	22.792	1896	1899	1902	rBV	195008	224244	23.16%	3.159%
21	24.335	2031	2034	2038	rBV3	8441	14909	1.54%	0.210%

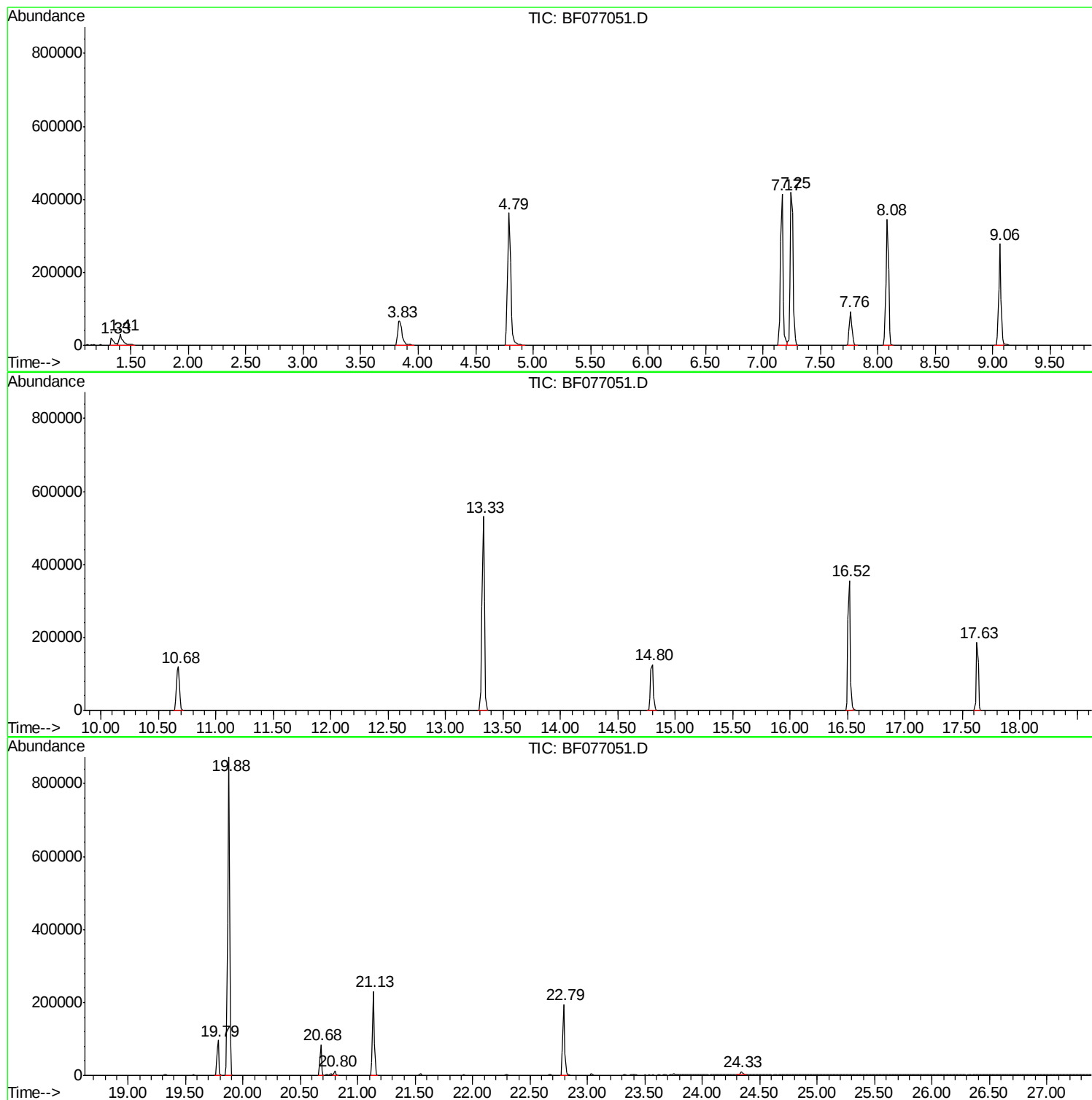
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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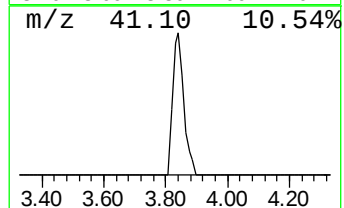
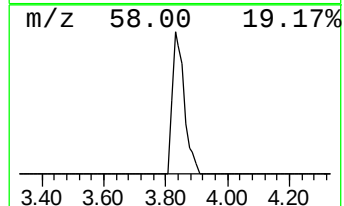
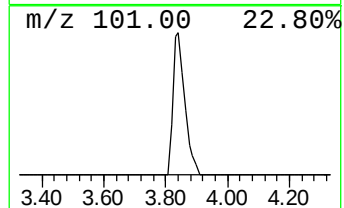
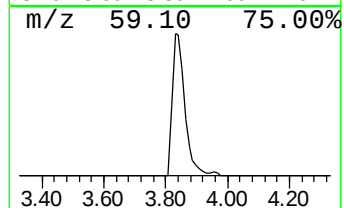
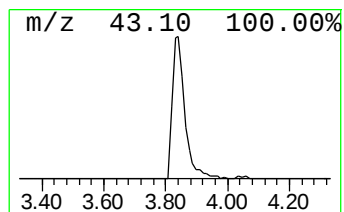
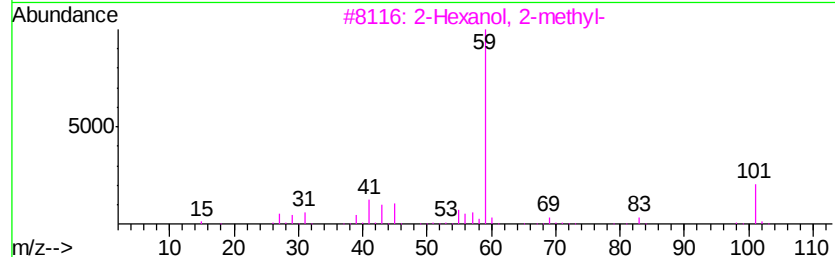
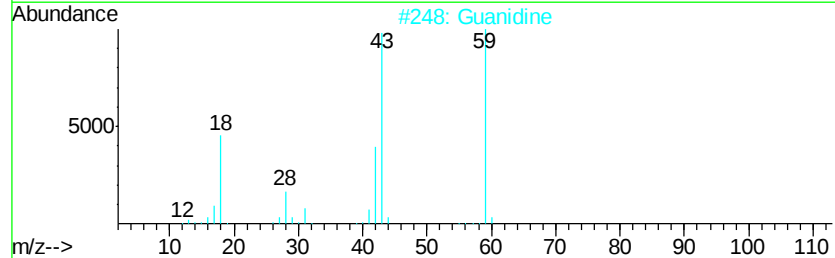
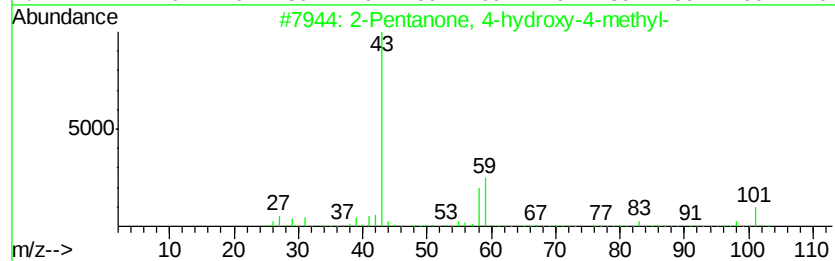
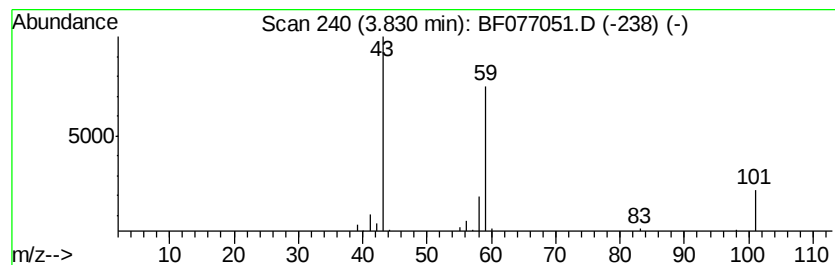
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.83	25.12 ng	182870	1,4-Dichlorobenzene-d4	7.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Guanidine	59	CH5N3	000113-00-8	47
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	36
5			Acetone	58	C3H6O	000067-64-1	9



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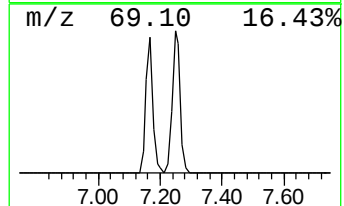
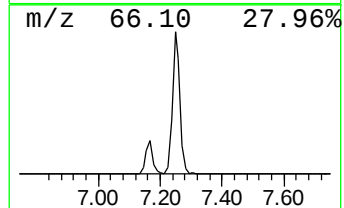
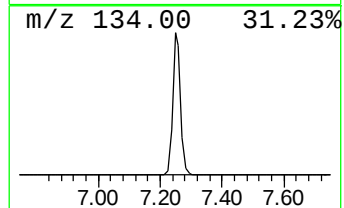
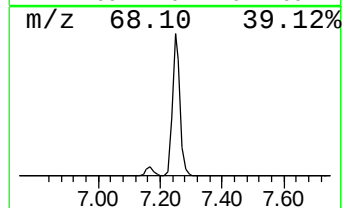
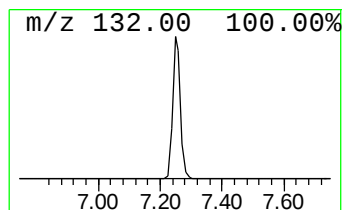
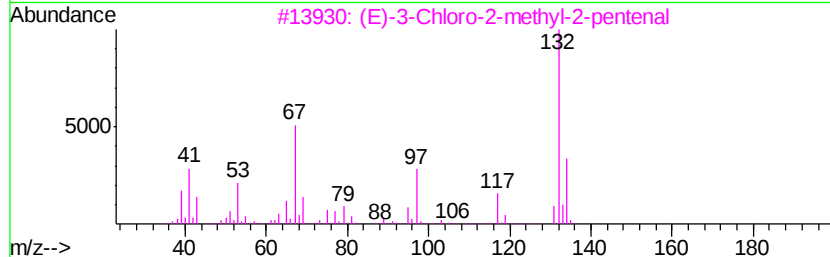
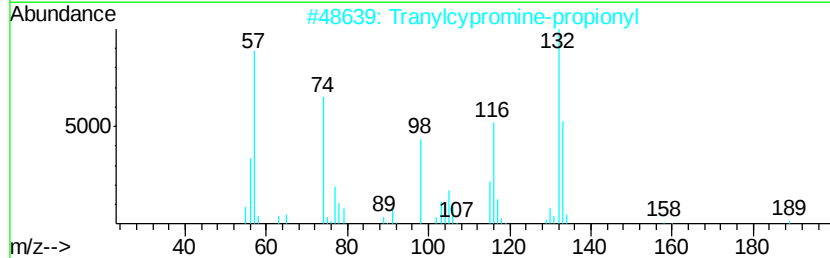
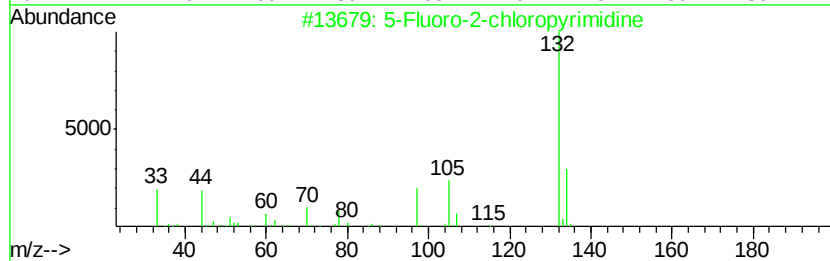
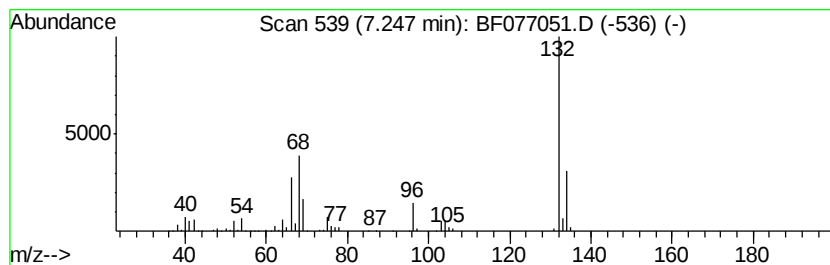
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Peak Number 4 unknown7.25 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.25	100.27 ng	729982	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



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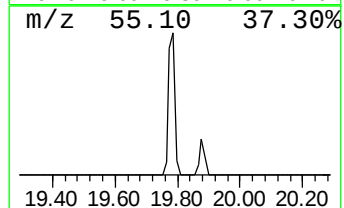
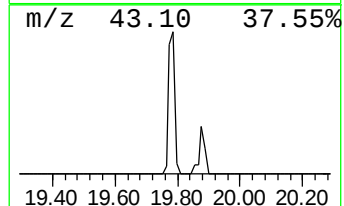
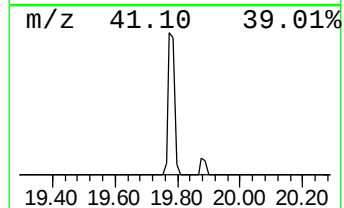
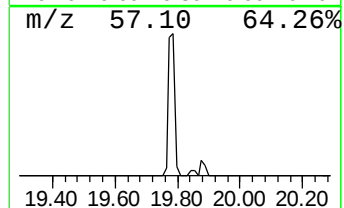
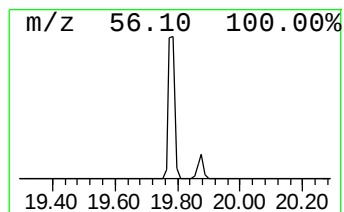
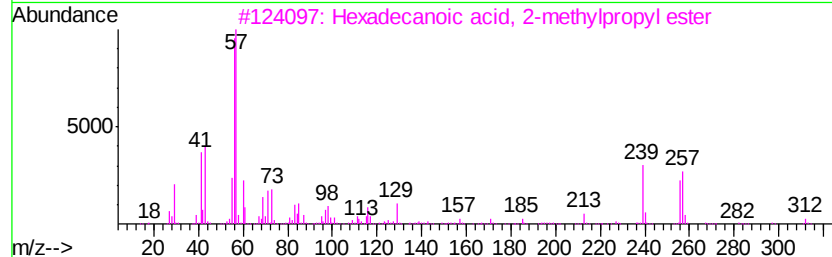
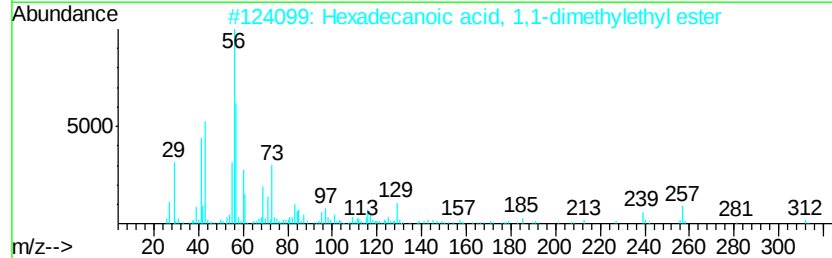
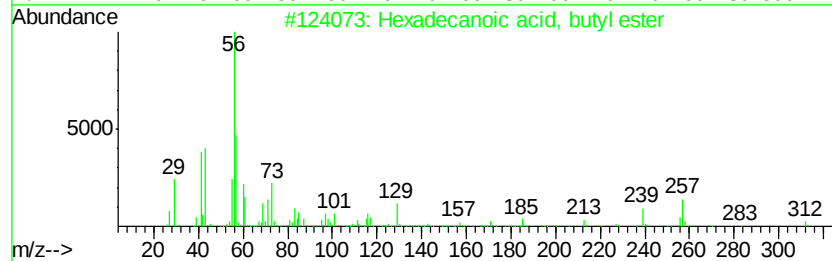
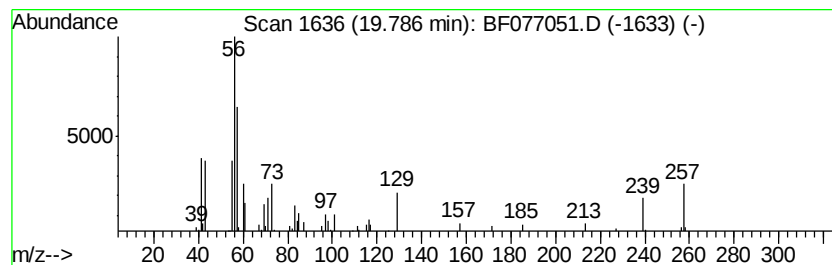
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.79	10.07 ng	124988	Chrysene-d12	21.13

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		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	59
4		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	27



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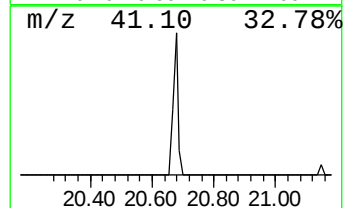
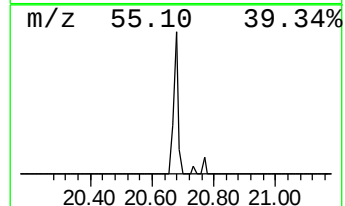
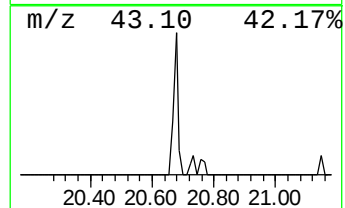
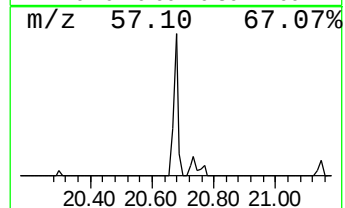
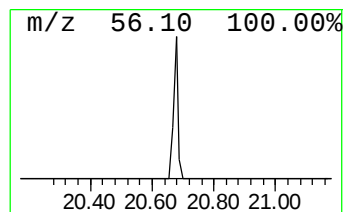
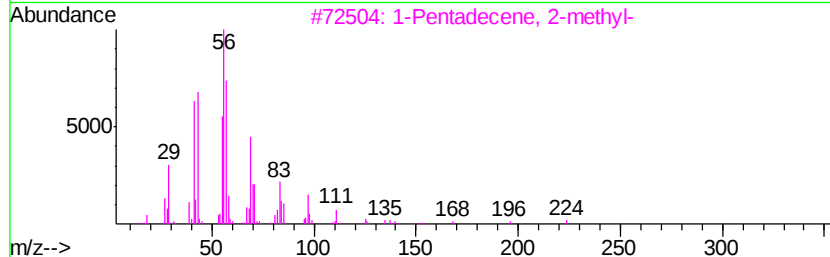
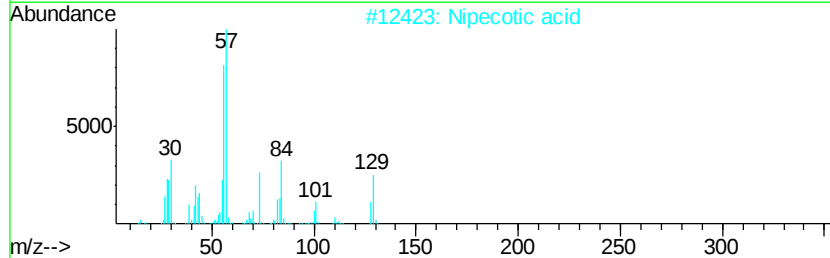
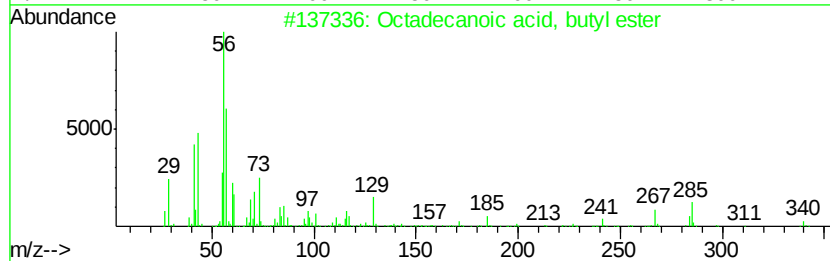
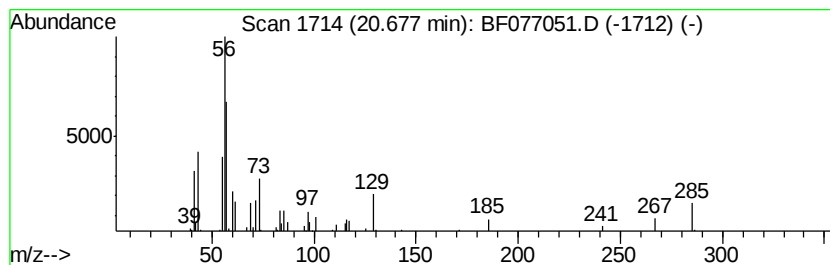
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Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.68	6.89 ng	85577	Chrysene-d12	21.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2			Nipecotic acid	129	C6H11NO2	000498-95-3	50
3			1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	32
4			Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5			2-Methyl-1-octadecene	266	C19H38	061868-20-0	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.83	25.1	ng	182870	1	7.76	145605	20.0
unknown7.25	7.25	100.3	ng	729982	1	7.76	145605	20.0
Hexadecanoic acid...	19.79	10.1	ng	124988	5	21.13	248271	20.0
Octadecanoic acid...	20.68	6.9	ng	85577	5	21.13	248271	20.0