

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041318\
 Data File : BF104521.D
 Acq On : 14 Apr 2018 12:27
 Operator : JU/SJ
 Sample : J2368-15
 Misc :
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 041118-SIDI-E-D-M

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-BF040618.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	5.004	492	496	504	rVB	160231	165989	3.81%	0.638%
2	5.422	563	567	570	rBV	1522960	1334453	30.60%	5.131%
3	6.034	668	671	677	rBV	60247	62964	1.44%	0.242%
4	6.439	736	740	748	rBV	901610	864735	19.83%	3.325%
5	6.575	759	763	767	rBV	2516524	2353912	53.98%	9.051%
6	6.804	799	802	806	rBV	1011198	880875	20.20%	3.387%
7	6.963	825	829	833	rBV	3197791	3216821	73.76%	12.369%
8	7.375	893	899	902	rBV	2583620	2650832	60.79%	10.192%
9	7.457	909	913	925	rVB	39843	51927	1.19%	0.200%
10	8.092	1017	1021	1024	rBV	1297657	1139325	26.13%	4.381%
11	9.169	1199	1204	1207	rBV	4396796	4360962	100.00%	16.768%
12	9.557	1267	1270	1279	rBV	308349	274608	6.30%	1.056%
13	9.845	1314	1319	1328	rVB	1359610	1190040	27.29%	4.576%
14	10.275	1384	1392	1395	rBV2	90426	84159	1.93%	0.324%
15	10.633	1449	1453	1464	rVB	1488196	1480627	33.95%	5.693%
16	10.745	1469	1472	1482	rVB	91269	91974	2.11%	0.354%
17	11.333	1568	1572	1576	rBV	1115363	931706	21.36%	3.582%
18	12.739	1808	1811	1815	rBV	129058	98664	2.26%	0.379%
19	12.927	1838	1843	1846	rBV	3134572	3072585	70.46%	11.814%
20	13.445	1928	1931	1935	rBV	79579	70466	1.62%	0.271%
21	13.815	1991	1994	2007	rBV	168244	206511	4.74%	0.794%
22	13.980	2018	2022	2029	rVB	841643	789763	18.11%	3.037%
23	15.439	2265	2270	2281	rVB	479939	634121	14.54%	2.438%

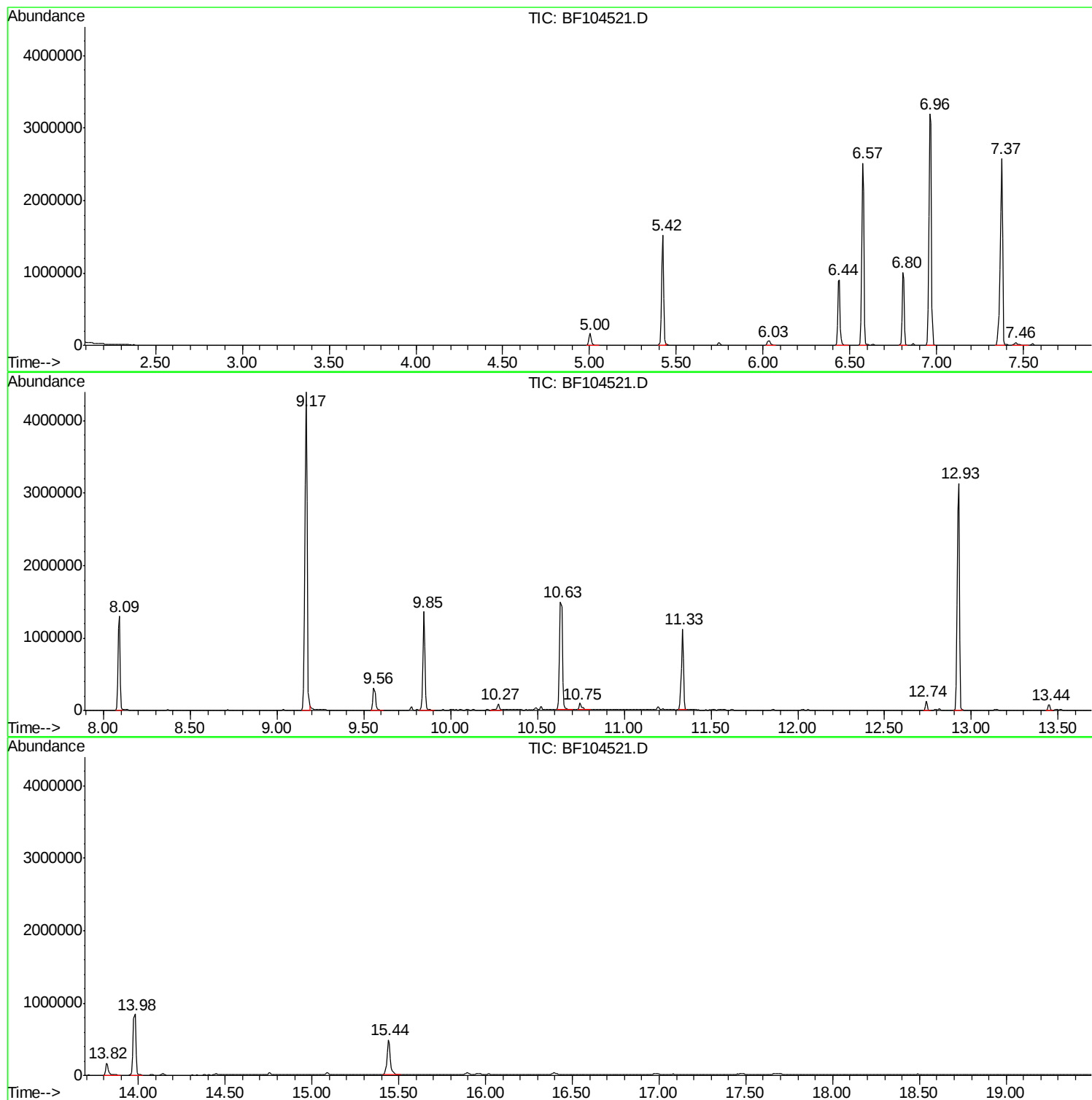
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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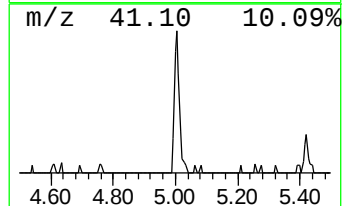
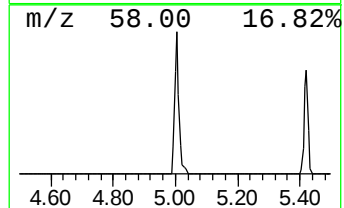
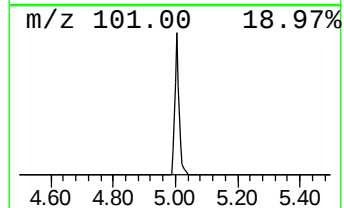
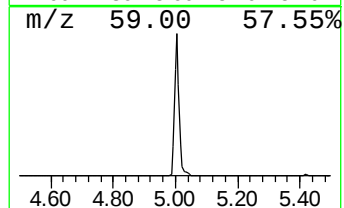
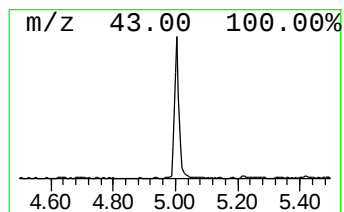
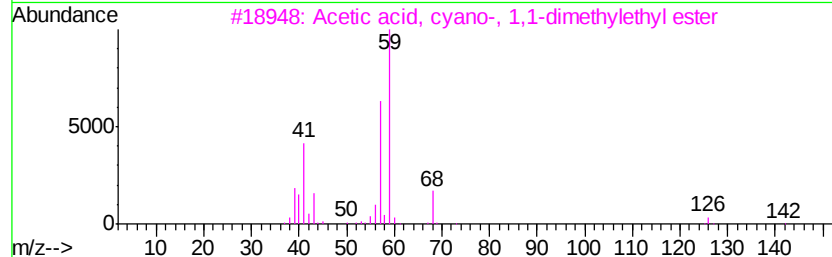
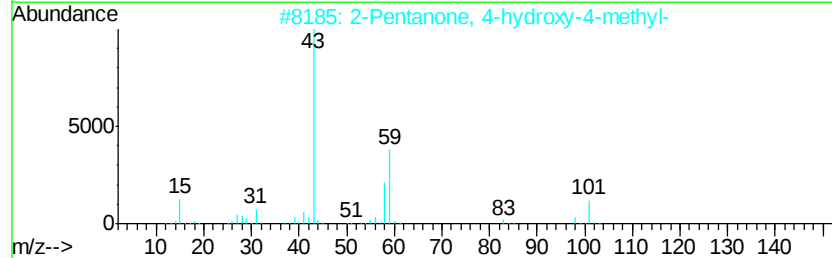
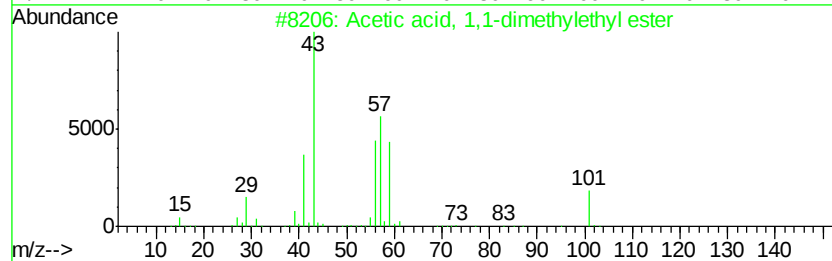
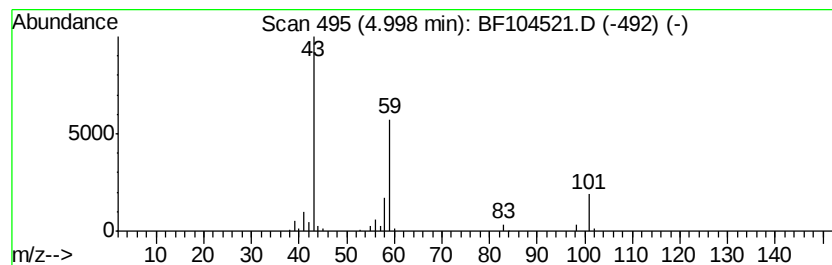
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetic acid, 1,1-dimethylet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.77 ng	165989	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3		Acetic acid, cyano-, 1,1-dimethv...	141	C7H11NO2	001116-98-9	23
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23



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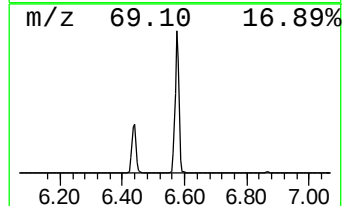
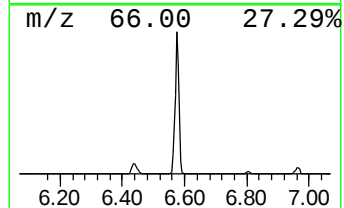
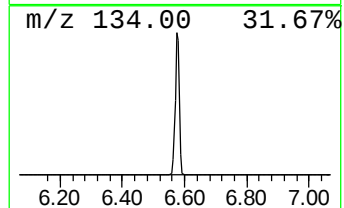
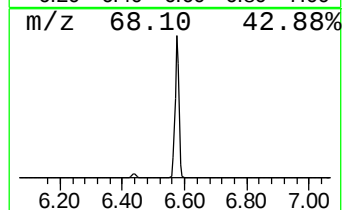
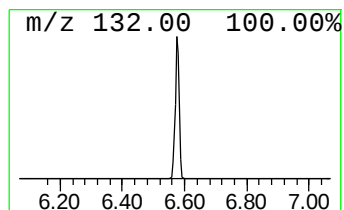
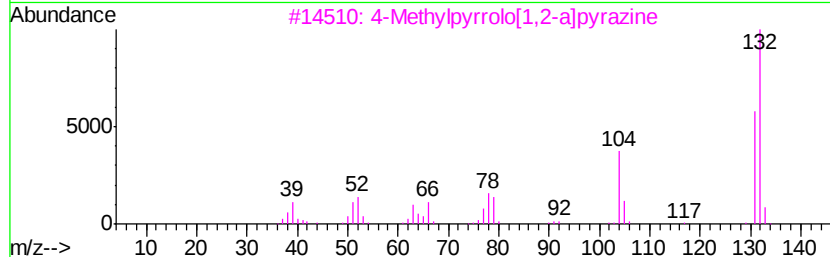
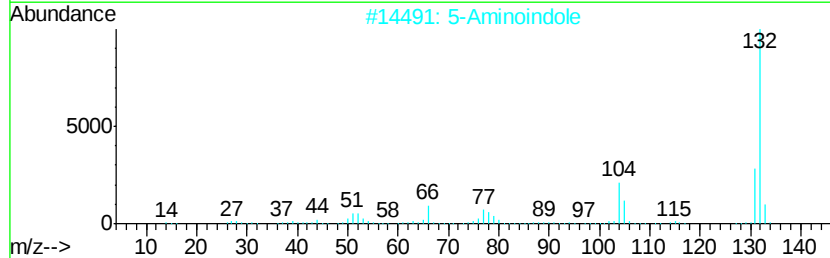
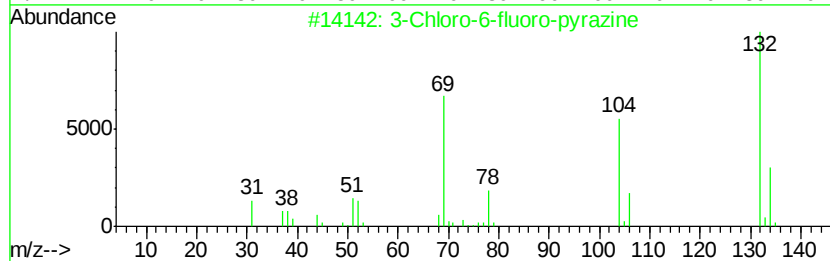
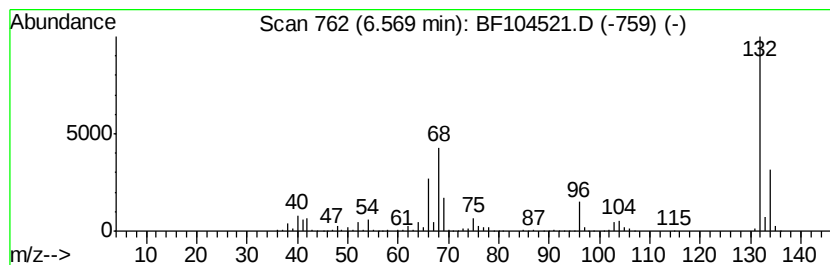
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Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	53.44 ng	2353910	1,4-Dichlorobenzene-d4	6.80

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			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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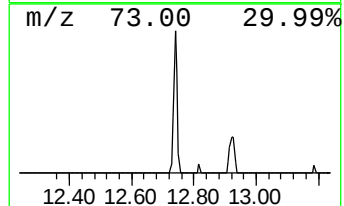
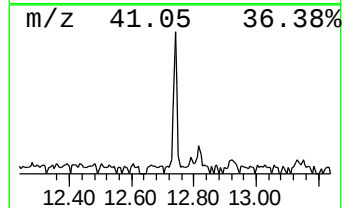
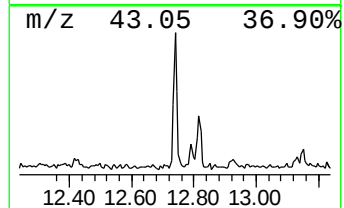
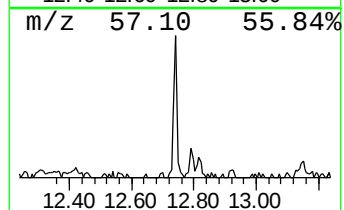
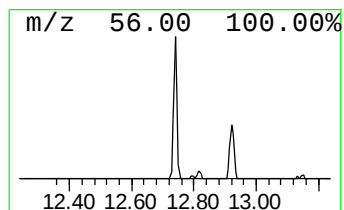
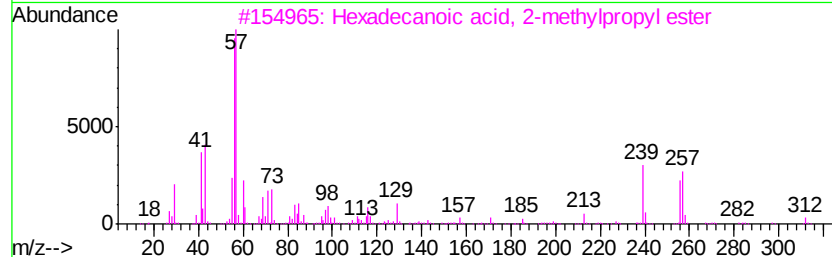
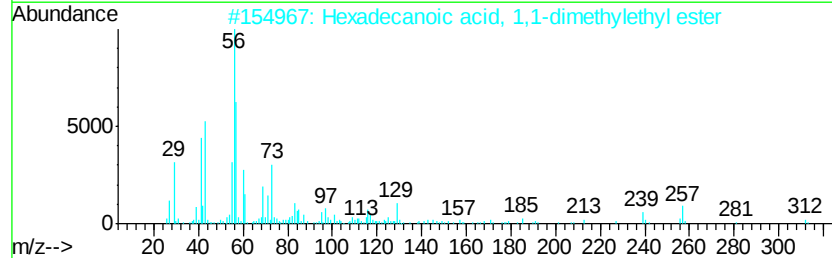
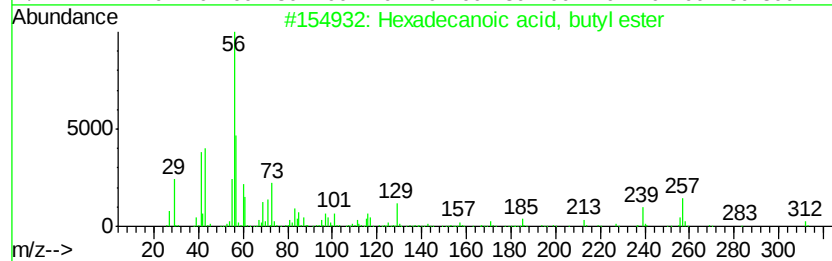
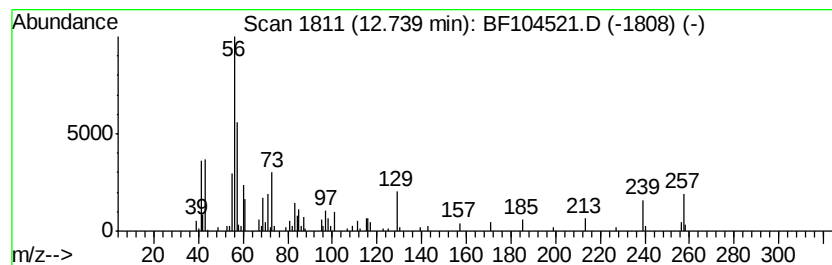
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.50 ng	98664	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	47
4		(n-Butylthio)acetonitrile	129	C6H11NS	071037-08-6	43
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



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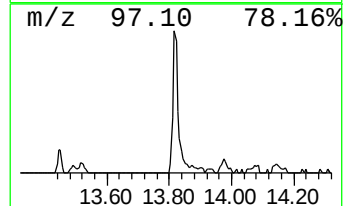
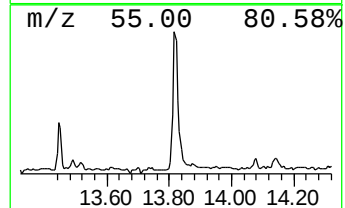
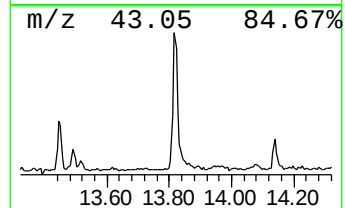
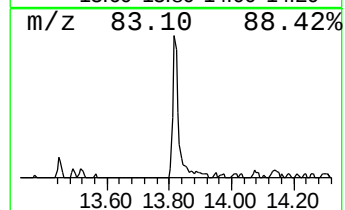
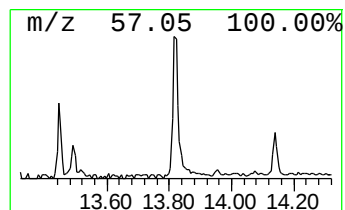
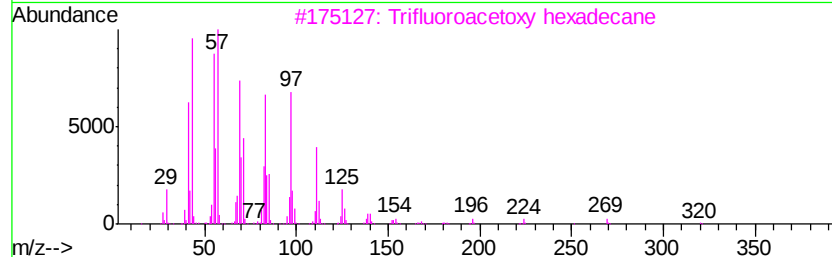
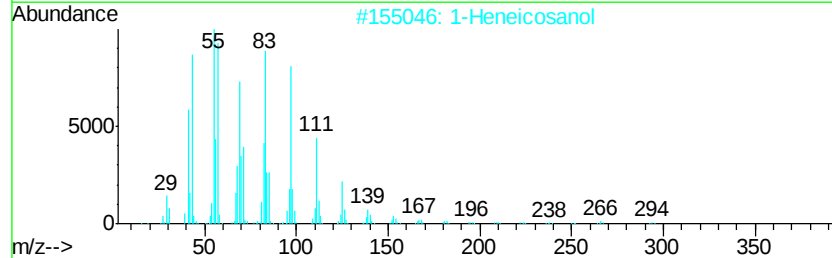
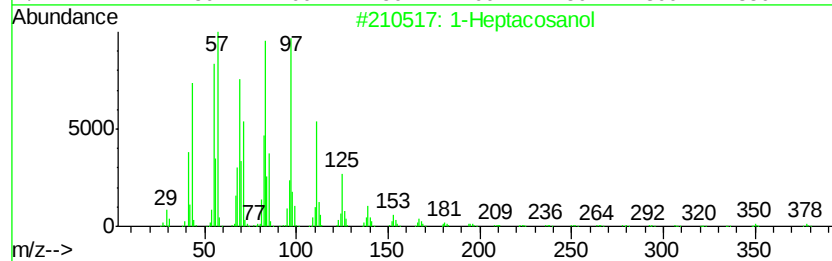
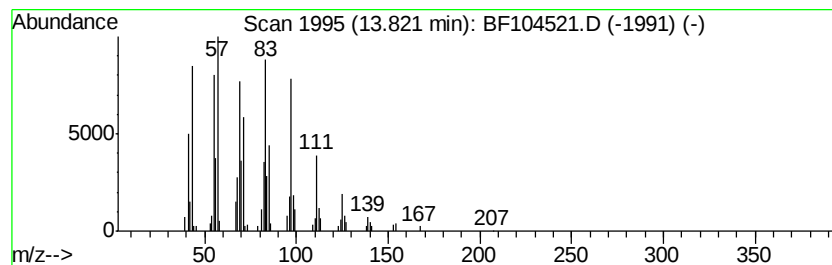
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Peak Number 5 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	5.23 ng	206511	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid, 1,1-...	5.00	3.8	ng	165989	1	6.80	880875	20.0
unknown6.57	6.57	53.4	ng	2353910	1	6.80	880875	20.0
Hexadecanoic acid...	12.74	2.5	ng	98664	5	13.98	789763	20.0
1-Heptacosanol	13.82	5.2	ng	206511	5	13.98	789763	20.0