

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111218\
 Data File : BF110717.D
 Acq On : 13 Nov 2018 11:43
 Operator : JU/SJ
 Sample : PB114706BL
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB114706BL

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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	5.181	522	526	541	rBV	45232	69086	3.27%	0.549%
2	5.563	588	591	609	rBV	1043847	1104849	52.25%	8.778%
3	6.563	757	761	780	rBV	1163388	1149185	54.35%	9.131%
4	6.710	782	786	794	rBV	1418013	1187368	56.15%	9.434%
5	6.939	822	825	837	rVB	389129	367058	17.36%	2.916%
6	7.098	848	852	867	rBV	1546697	1370610	64.82%	10.890%
7	7.510	917	922	935	rBV	1001785	1077754	50.97%	8.563%
8	8.228	1040	1044	1057	rBV	438015	507587	24.00%	4.033%
9	9.298	1221	1226	1242	rBV	2407672	2114524	100.00%	16.800%
10	9.986	1339	1343	1355	rBV	508246	548978	25.96%	4.362%
11	10.775	1474	1477	1492	rBV	532935	577986	27.33%	4.592%
12	11.480	1593	1597	1610	rBV	428575	482203	22.80%	3.831%
13	12.857	1828	1831	1835	rBV	41055	36930	1.75%	0.293%
14	13.057	1861	1865	1869	rBV	1491973	1330949	62.94%	10.575%
15	14.127	2043	2047	2057	rBV	331857	340065	16.08%	2.702%
16	15.615	2296	2300	2303	rBV2	20655	27374	1.29%	0.217%
17	15.657	2303	2307	2318	rVB	171684	264083	12.49%	2.098%
18	16.074	2372	2378	2384	rBV2	16018	29555	1.40%	0.235%

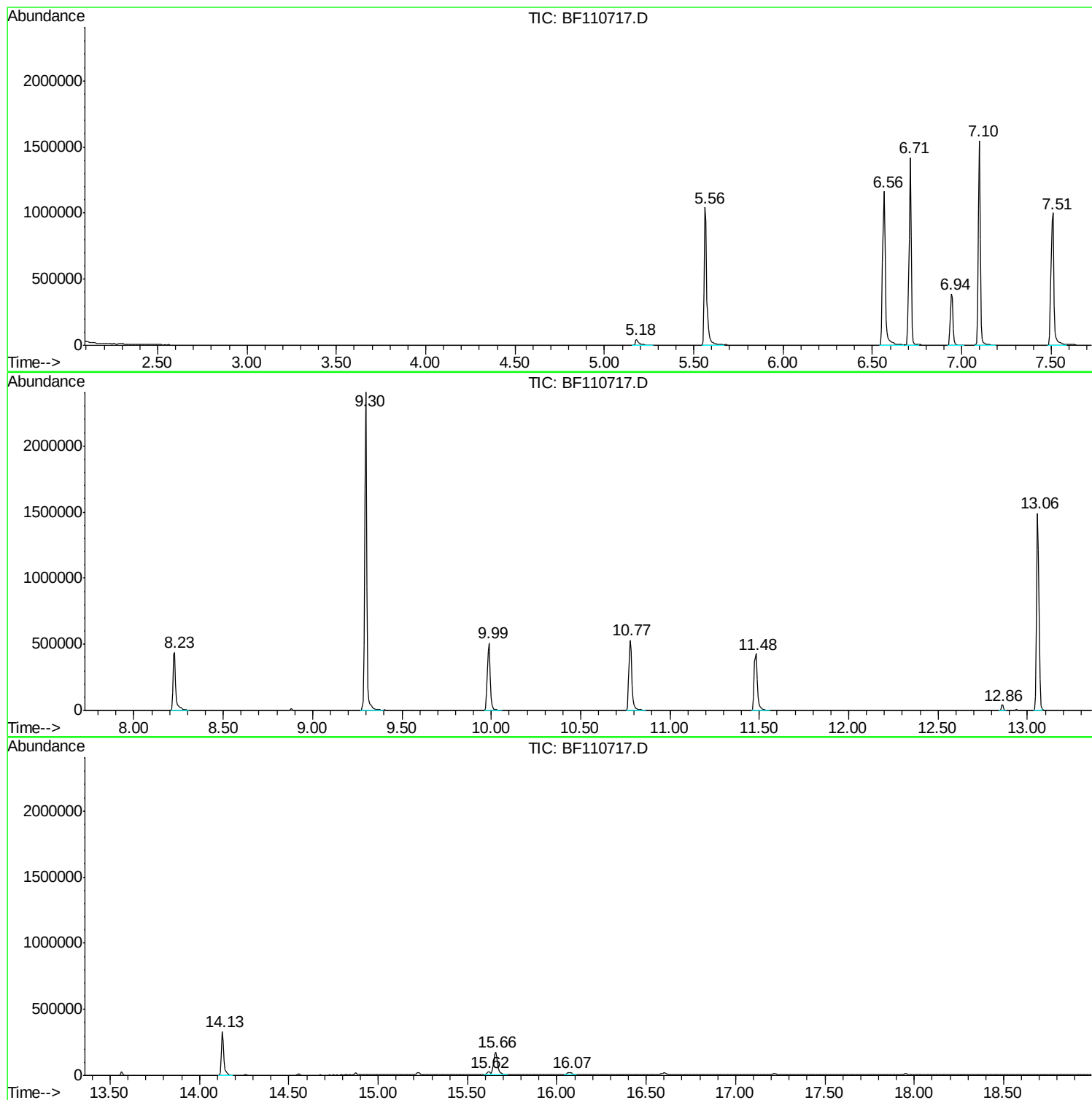
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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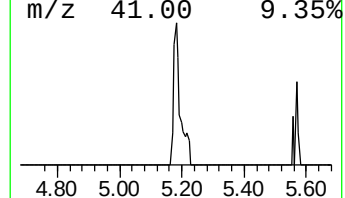
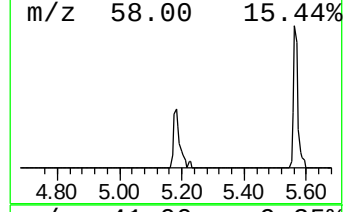
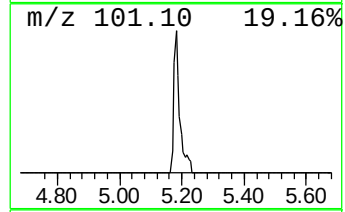
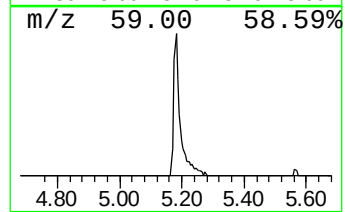
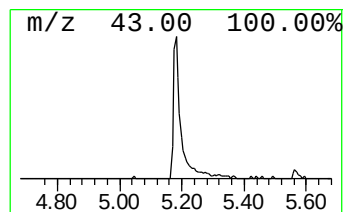
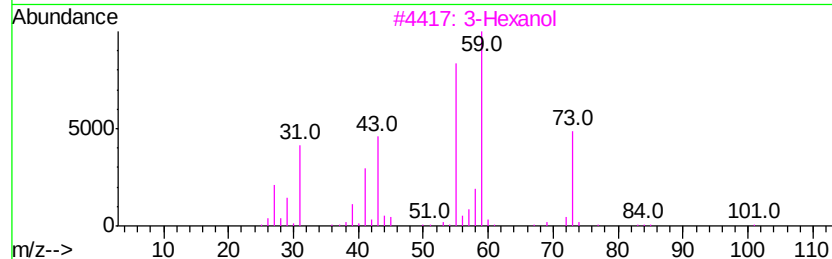
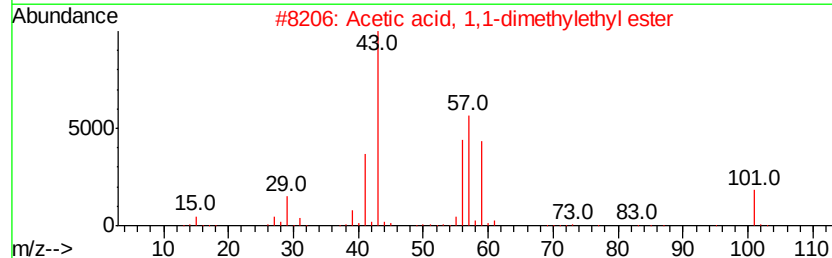
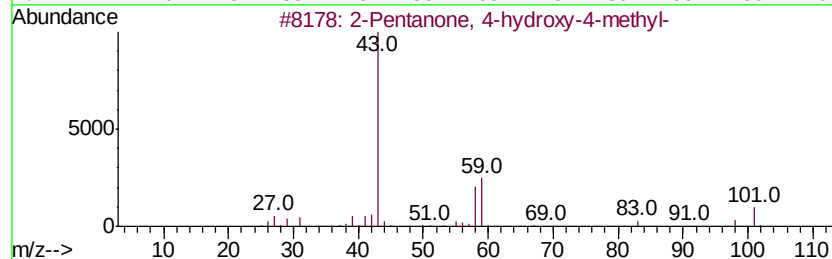
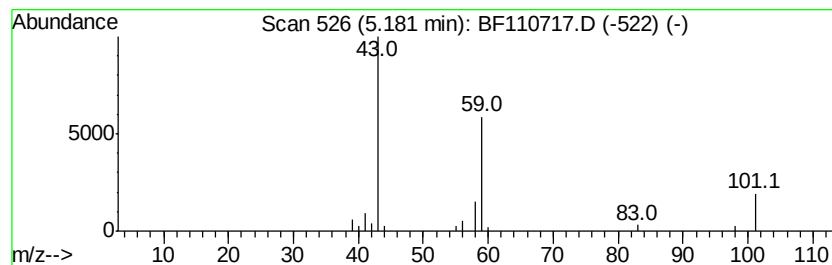
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	3.76 ng	69086	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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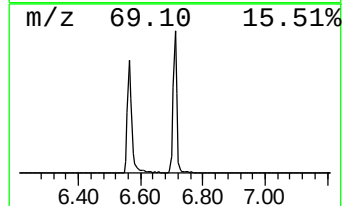
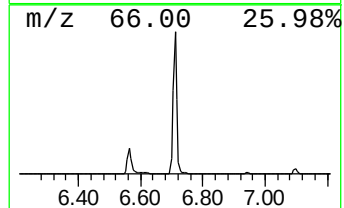
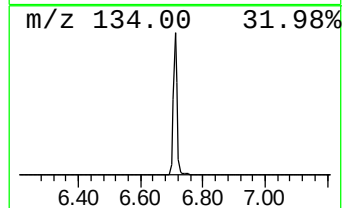
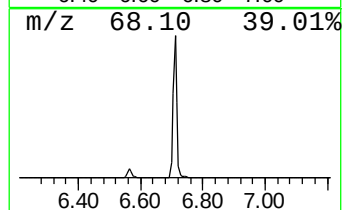
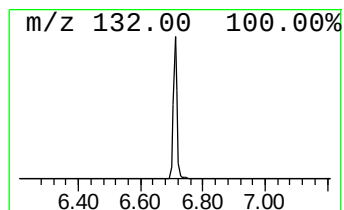
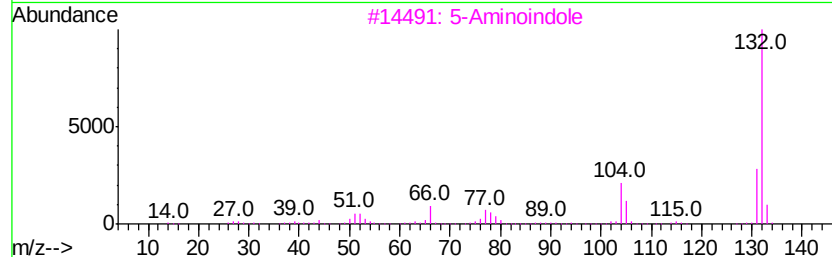
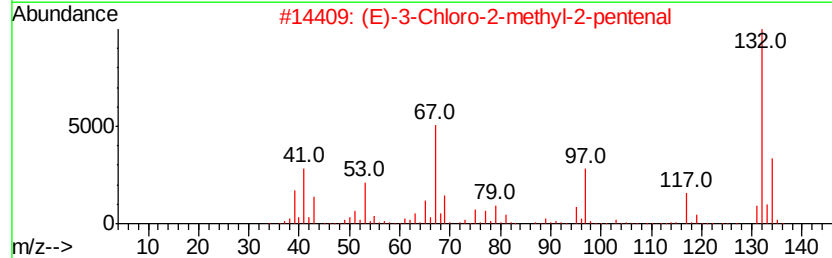
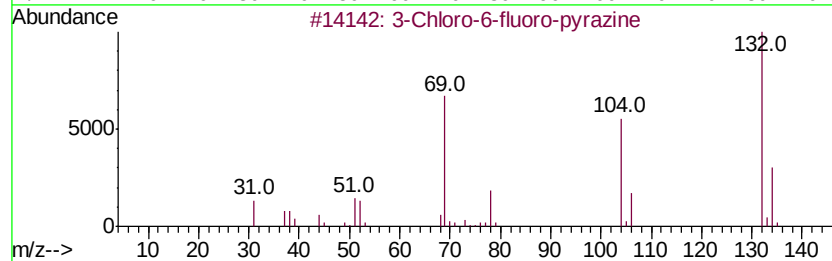
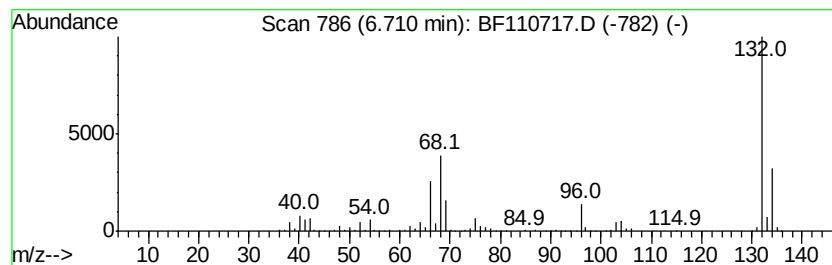
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Peak Number 2 unknown6.71 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	64.70 ng	1187370	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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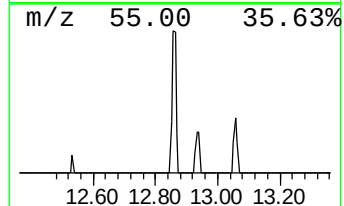
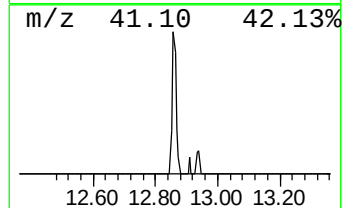
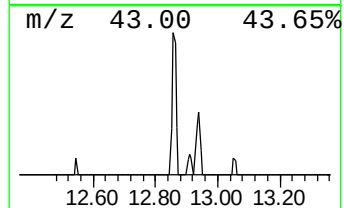
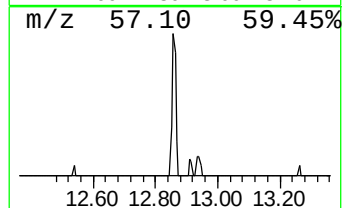
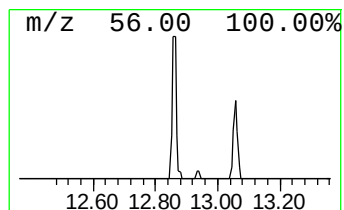
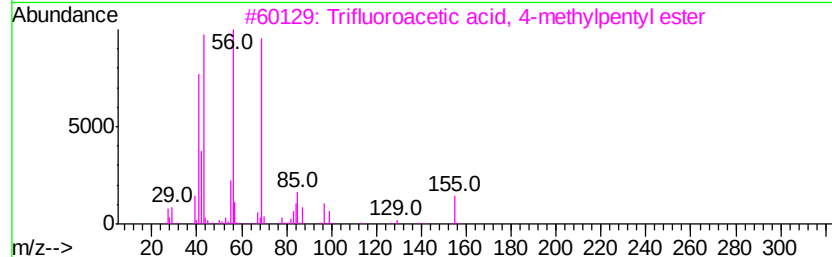
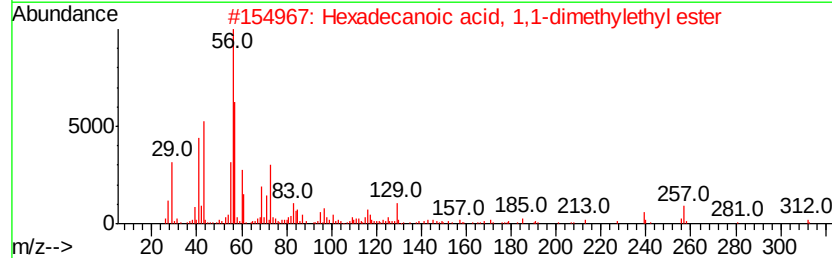
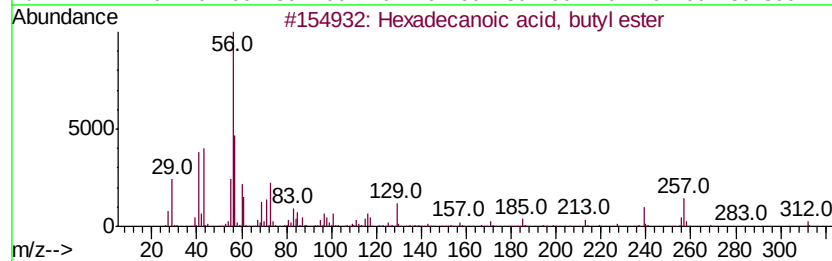
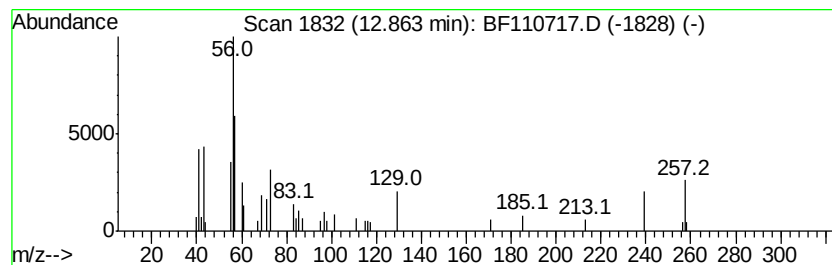
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	2.17 ng	36930	Chrysene-d12	14.13

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	80
3		Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	32
4		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	32
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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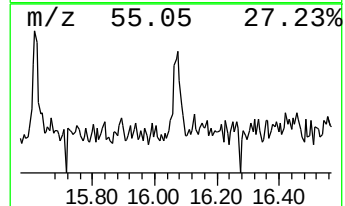
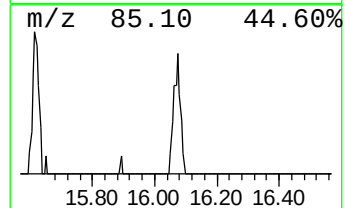
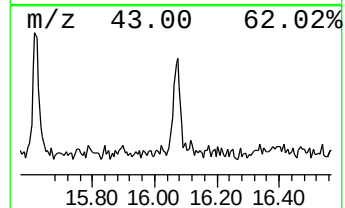
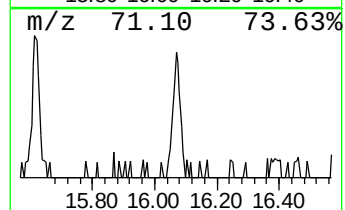
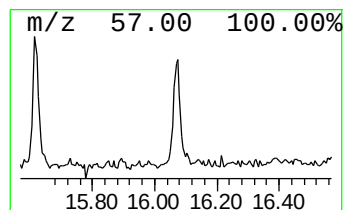
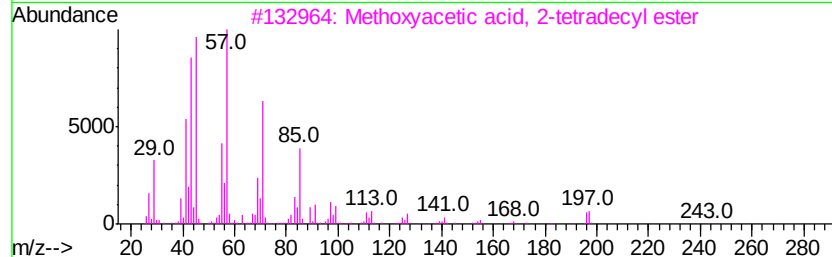
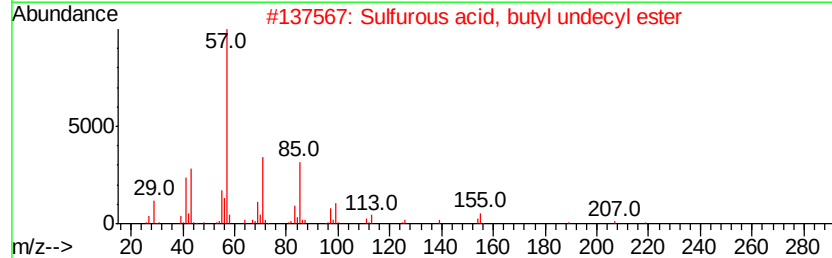
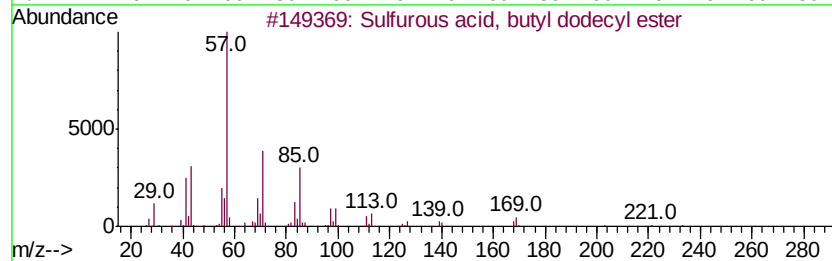
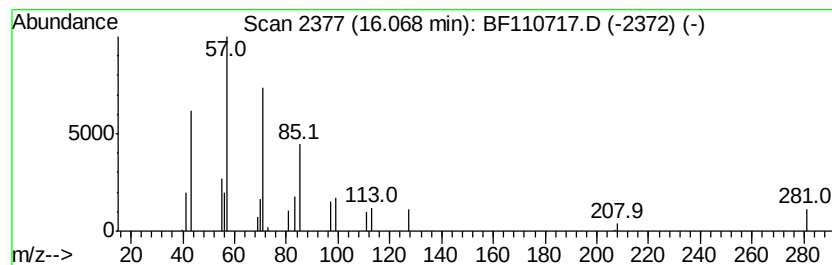
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Peak Number 5 Sulfurous acid, butyl dodec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.24 ng	29555	Perylene-d12	15.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	78
2		Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	78
3		Methoxvacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	72
4		Heneicosane	296	C21H44	000629-94-7	72
5		Tetrapentacontane	759	C54H110	005856-66-6	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	3.8	ng	69086	1	6.95	367058	20.0
unknown6.71	6.71	64.7	ng	1187370	1	6.95	367058	20.0
Hexadecanoic acid...	12.86	2.2	ng	36930	5	14.13	340065	20.0
Sulfurous acid, b...	16.07	2.2	ng	29555	6	15.66	264083	20.0