

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062118\
 Data File : BF106671.D
 Acq On : 21 Jun 2018 20:01
 Operator : JU/SJ
 Sample : J3554-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-3(5.0)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.207	484	488	497	rBV	122210	156602	8.24%	0.889%
2	5.607	552	556	560	rBV	1562646	1537739	80.93%	8.727%
3	6.607	721	726	729	rBV	1478877	1628445	85.70%	9.242%
4	6.742	744	749	752	rBV	1607616	1604951	84.46%	9.108%
5	6.960	782	786	789	rVB	485428	387583	20.40%	2.200%
6	7.119	808	813	816	rBV	1417117	1311194	69.00%	7.441%
7	7.525	876	882	885	rBV	1070812	1116910	58.78%	6.339%
8	7.983	957	960	963	rBB	66007	49867	2.62%	0.283%
9	8.242	1000	1004	1007	rBV	597423	503464	26.50%	2.857%
10	8.860	1104	1109	1112	rBV	1440661	1294810	68.14%	7.348%
11	9.319	1181	1187	1190	rBV	1936625	1886949	99.30%	10.709%
12	9.707	1249	1253	1256	rBV	445031	348193	18.32%	1.976%
13	10.001	1299	1303	1307	rBV	690508	585114	30.79%	3.321%
14	10.413	1370	1373	1375	rVB	45665	35862	1.89%	0.204%
15	10.795	1433	1438	1442	rBV	1312712	1337275	70.38%	7.589%
16	10.883	1450	1453	1457	rBV	49036	46406	2.44%	0.263%
17	11.330	1527	1529	1532	rBV	22857	19611	1.03%	0.111%
18	11.495	1553	1557	1560	rBV	665404	621186	32.69%	3.525%
19	12.877	1789	1792	1796	rBV2	42366	33928	1.79%	0.193%
20	13.077	1821	1826	1829	rBV	1904538	1900187	100.00%	10.784%
21	13.583	1909	1912	1915	rBV	23506	19045	1.00%	0.108%
22	13.954	1972	1975	1985	rBV	124366	137584	7.24%	0.781%
23	14.142	2003	2007	2011	rBV	531368	468191	24.64%	2.657%
24	14.601	2082	2085	2091	rBV4	25545	35674	1.88%	0.202%
25	15.683	2264	2269	2277	rBV	393955	496798	26.14%	2.819%
26	16.136	2342	2346	2351	rVB2	27510	31827	1.67%	0.181%
27	16.671	2433	2437	2441	rBV6	15668	25101	1.32%	0.142%

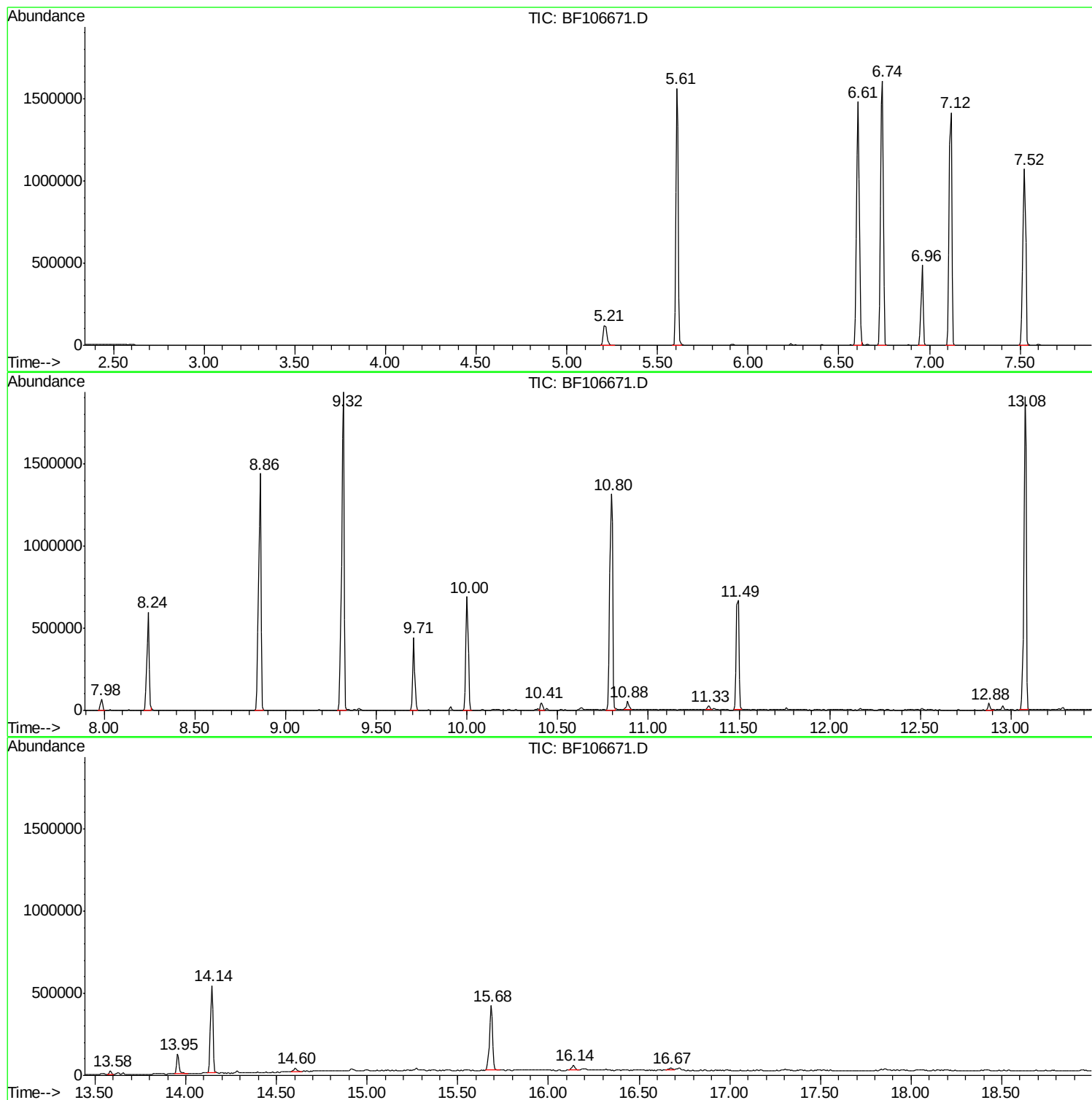
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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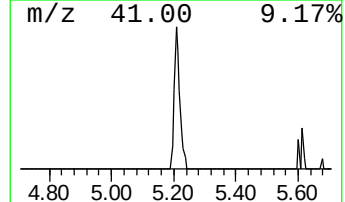
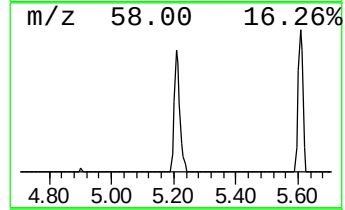
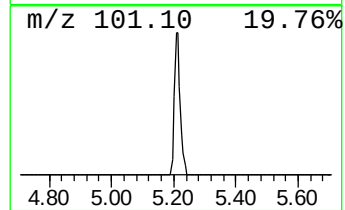
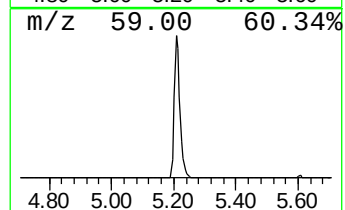
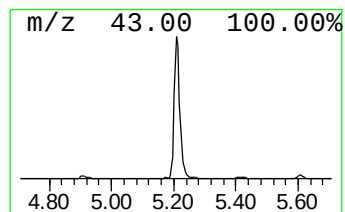
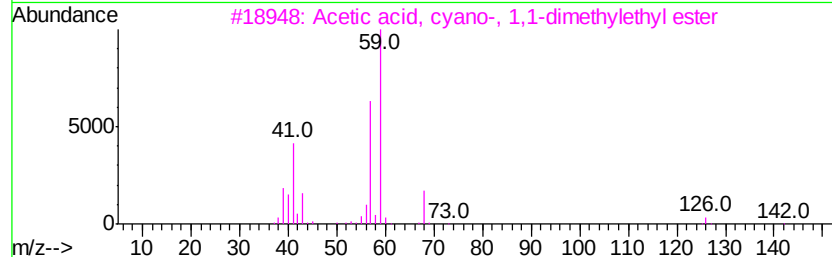
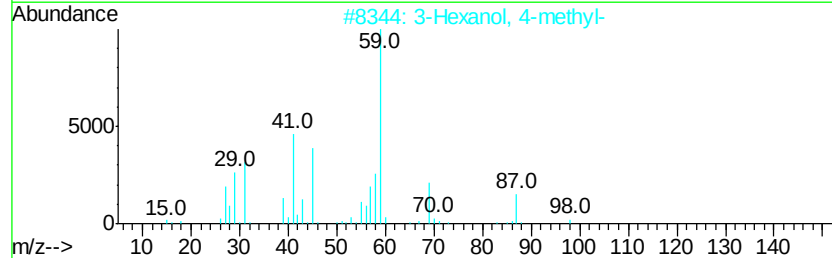
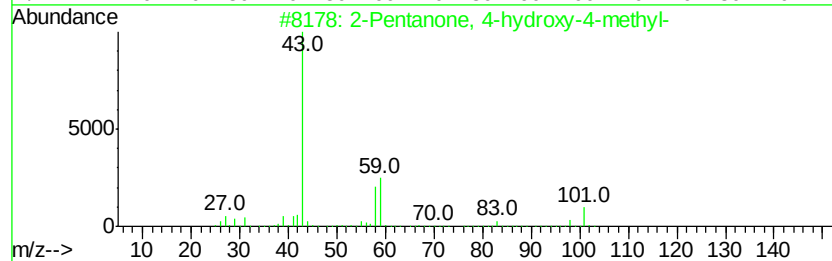
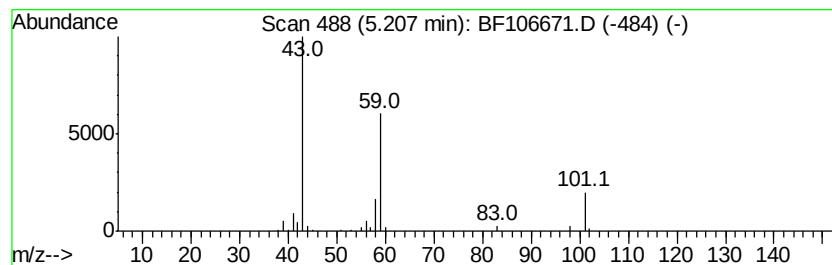
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	8.08 ng	156602	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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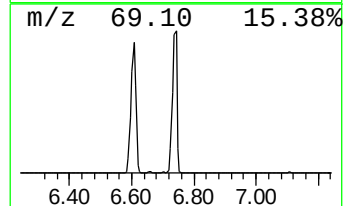
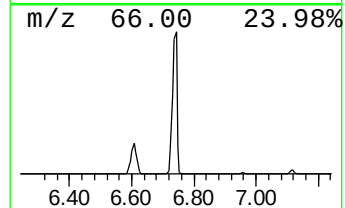
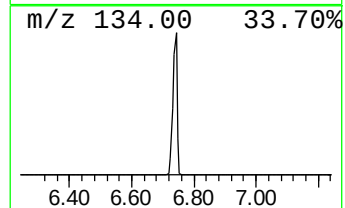
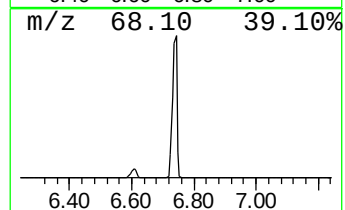
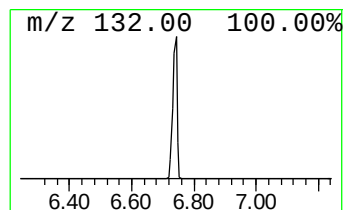
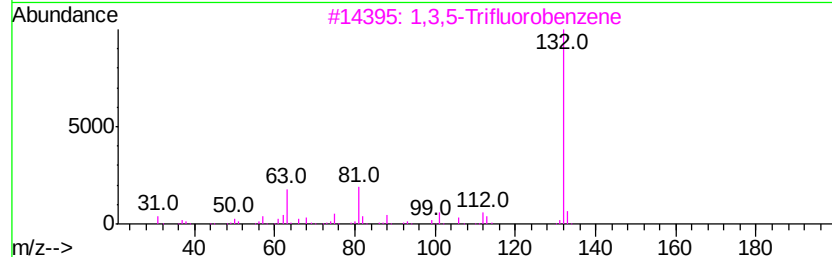
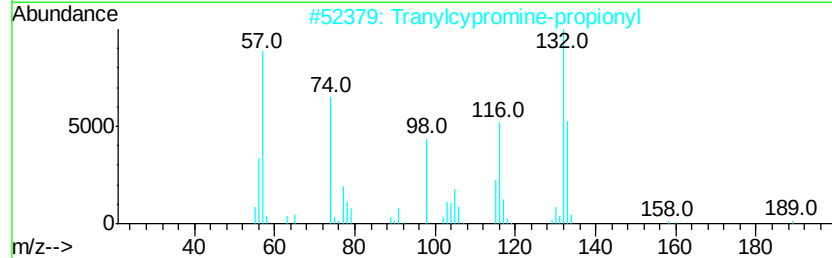
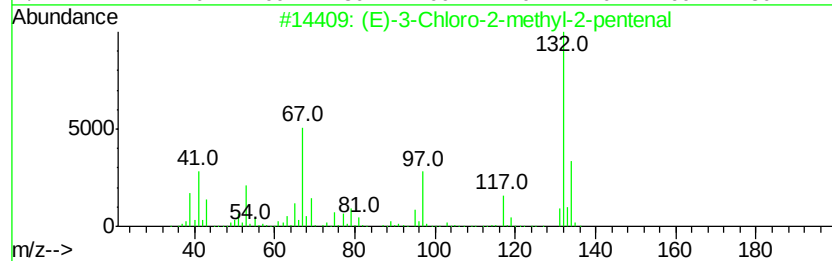
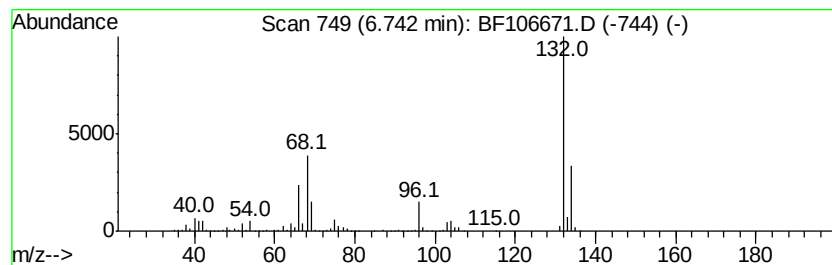
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	82.82 ng	1604950	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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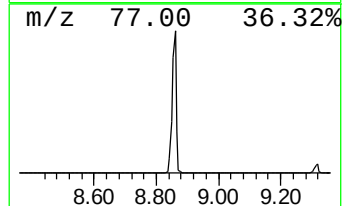
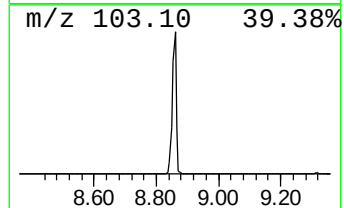
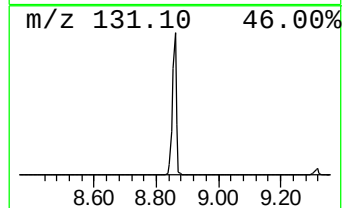
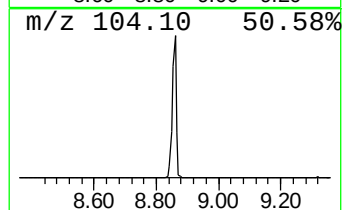
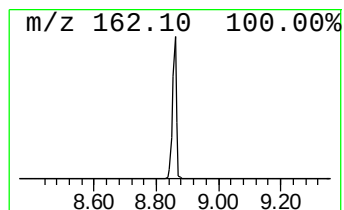
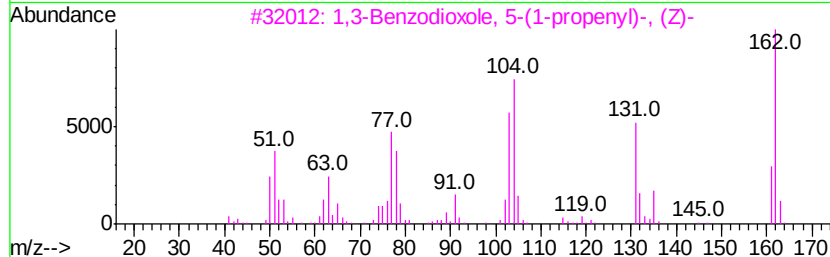
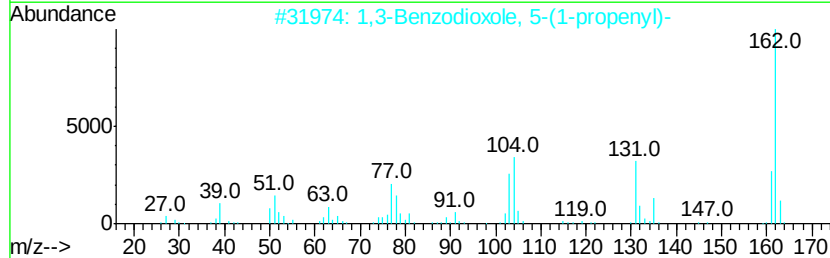
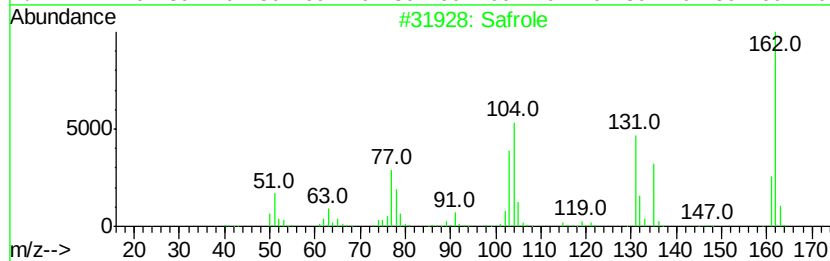
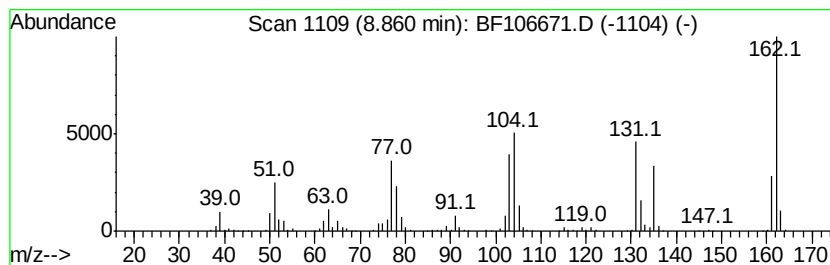
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Peak Number 4 Safrole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.86	51.44 ng	1294810	Napthalene-d8	8.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Safrole	162	C10H10O2	000094-59-7	98
2		1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3		1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	94
4		Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	94
5		1,4-Dioxo-1,2,3,4-tetrahydrophth...	162	C8H6N2O2	001445-69-8	45



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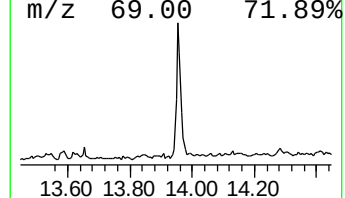
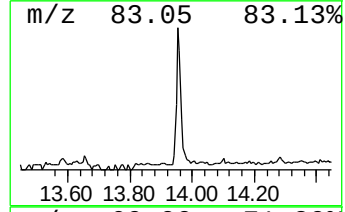
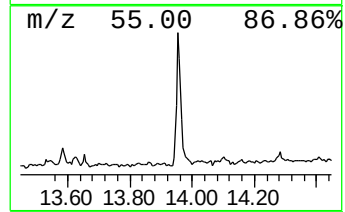
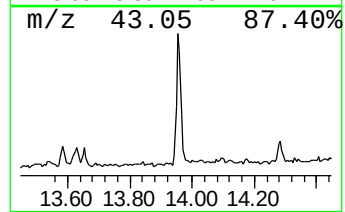
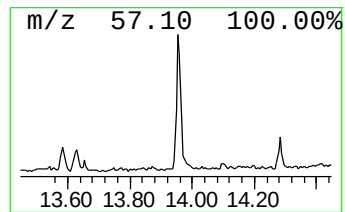
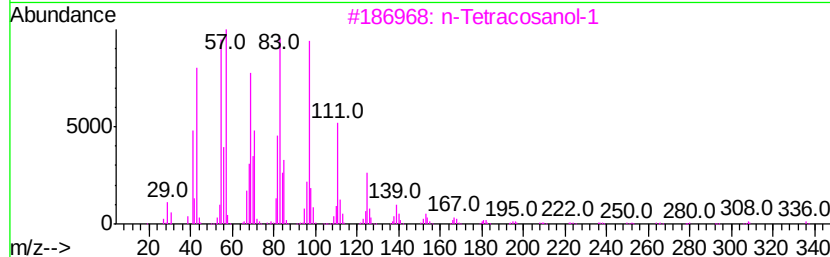
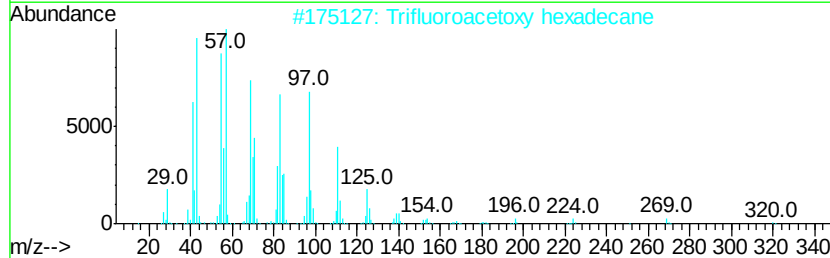
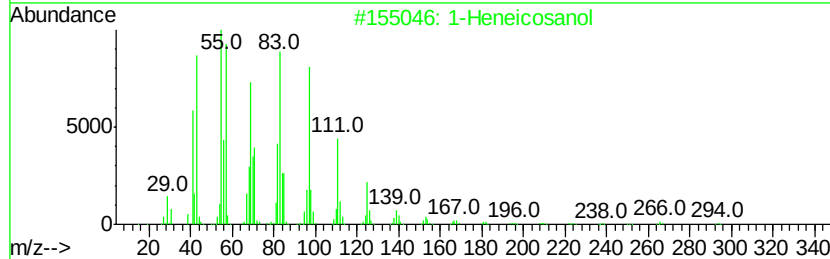
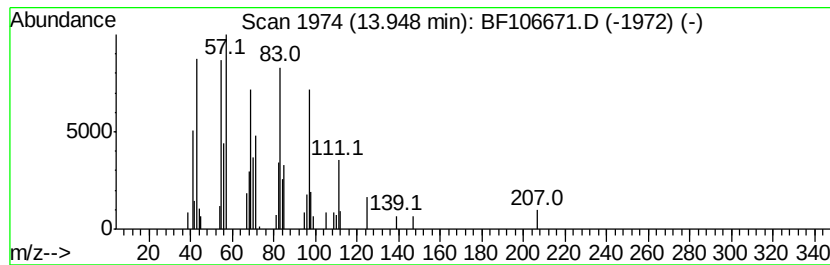
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.95	5.88 ng	137584	Chrysene-d12		14.14
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	8.1	ng	156602	1	6.96	387583	20.0
unknown6.74	6.74	82.8	ng	1604950	1	6.96	387583	20.0
Safrole	8.86	51.4	ng	1294810	2	8.24	503464	20.0
1-Heneicosanol	13.95	5.9	ng	137584	5	14.14	468191	20.0