

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
 Data File : BF108975.D
 Acq On : 13 Sep 2018 20:10
 Operator : JU/SJ
 Sample : J4875-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091118-JETT-F-U-B

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-BF090518.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	4.907	434	437	448	rVB	105499	116696	2.86%	0.445%
2	5.331	505	509	513	rBV	1416561	1253772	30.78%	4.781%
3	6.354	679	683	692	rBV	1094619	884705	21.72%	3.374%
4	6.495	702	707	710	rBV	2594342	2214100	54.35%	8.443%
5	6.725	743	746	750	rBV	900395	798838	19.61%	3.046%
6	6.884	769	773	777	rBV	2950735	2841397	69.75%	10.836%
7	7.289	837	842	845	rBV	2689117	2430773	59.67%	9.270%
8	8.007	960	964	968	rBV	1178535	974262	23.92%	3.715%
9	9.089	1143	1148	1151	rBV	4462737	4073745	100.00%	15.535%
10	9.478	1210	1214	1217	rBV	415305	314268	7.71%	1.198%
11	9.760	1258	1262	1265	rBV	1238909	1053696	25.87%	4.018%
12	10.436	1374	1377	1381	rVB	64302	53198	1.31%	0.203%
13	10.542	1391	1395	1398	rBV	1873183	1639403	40.24%	6.252%
14	11.236	1509	1513	1516	rBV	1180576	960846	23.59%	3.664%
15	11.771	1601	1604	1615	rBV2	65658	79033	1.94%	0.301%
16	12.818	1778	1782	1786	rBV	3603912	3658152	89.80%	13.950%
17	13.742	1934	1939	1953	rBV3	49270	155984	3.83%	0.595%
18	13.860	1955	1959	1963	rVB	1059094	917523	22.52%	3.499%
19	14.648	2089	2093	2097	rBV	74223	71788	1.76%	0.274%
20	14.718	2101	2105	2111	rVB	214093	202423	4.97%	0.772%
21	14.965	2143	2147	2153	rBV	78156	88677	2.18%	0.338%
22	15.271	2193	2199	2203	rBV	847987	1001461	24.58%	3.819%
23	15.324	2204	2208	2215	rVB	93580	119374	2.93%	0.455%
24	15.730	2272	2277	2283	rBV	104507	141949	3.48%	0.541%
25	16.201	2352	2357	2366	rVB	69403	119724	2.94%	0.457%
26	16.748	2445	2450	2456	rVB4	29903	57104	1.40%	0.218%

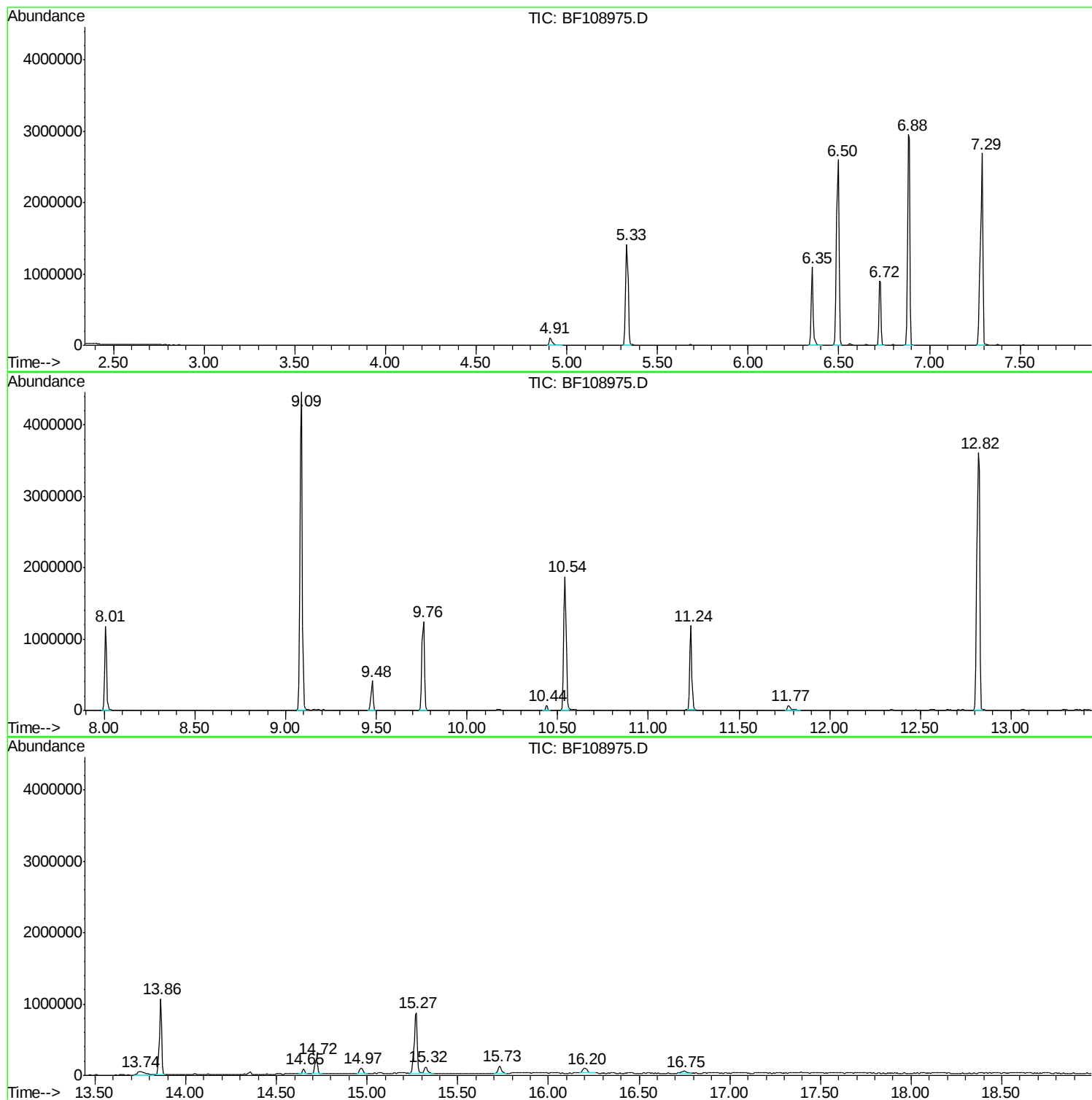
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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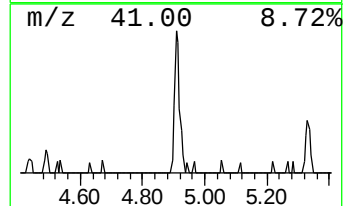
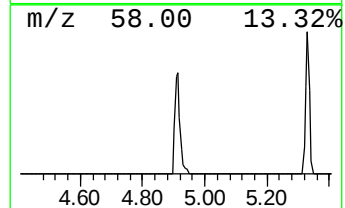
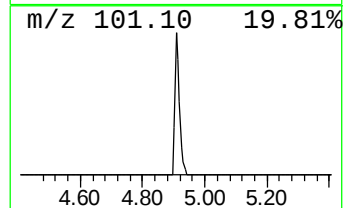
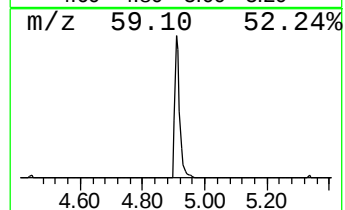
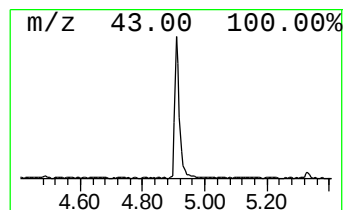
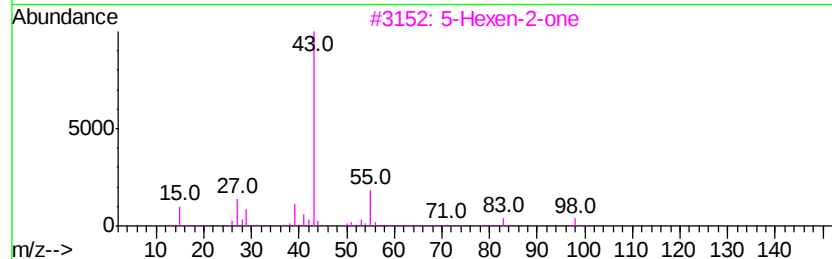
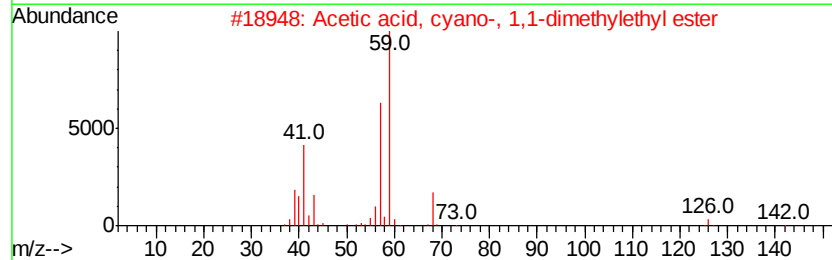
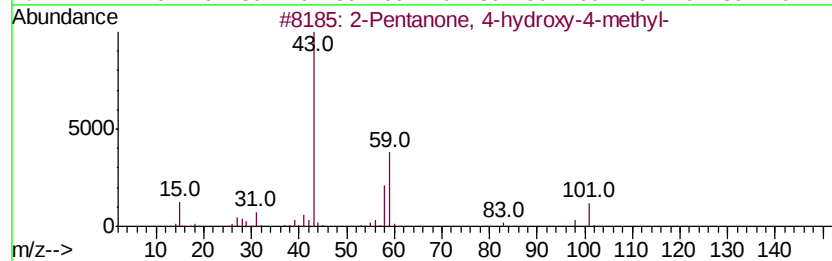
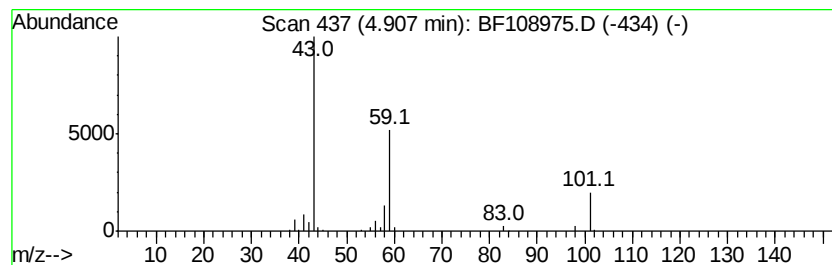
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	2.92 ng	116696	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9



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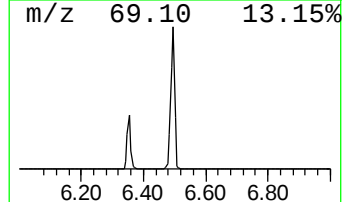
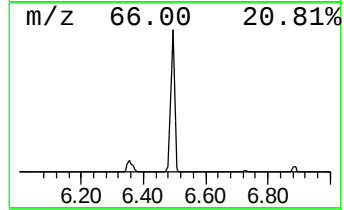
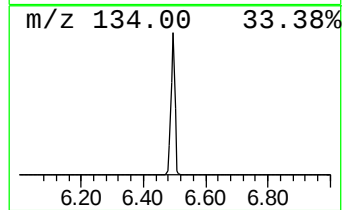
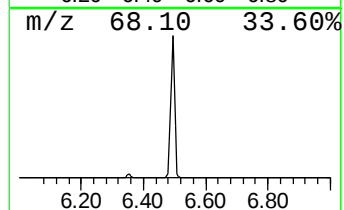
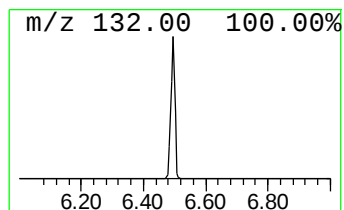
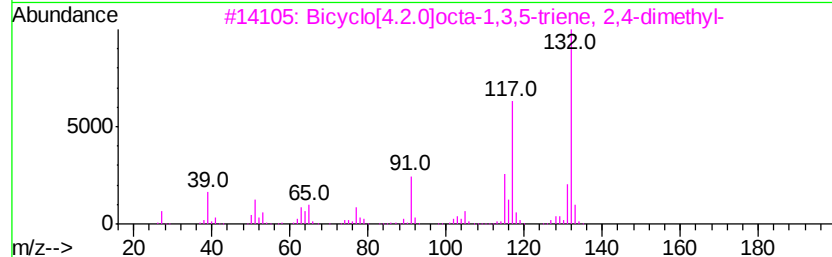
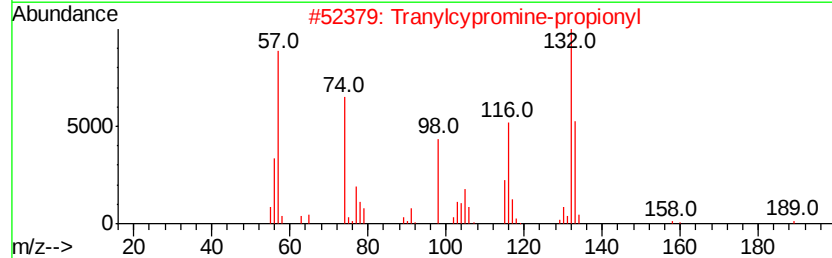
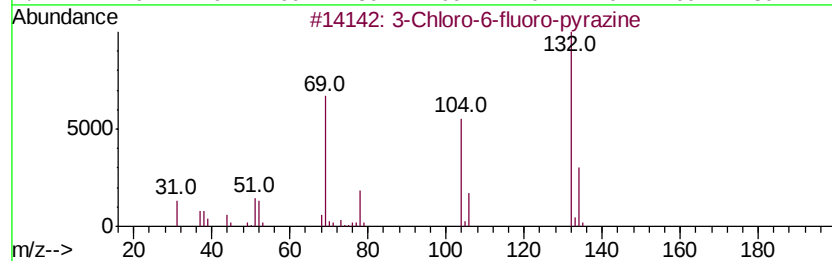
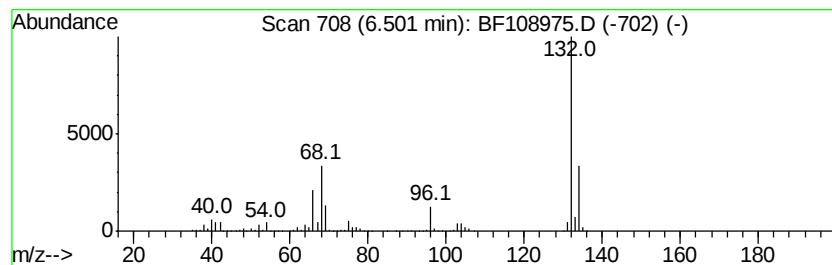
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Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	55.43 ng	2214100	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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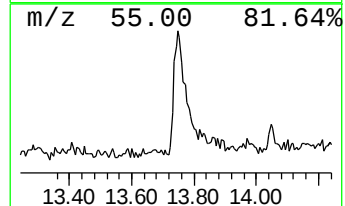
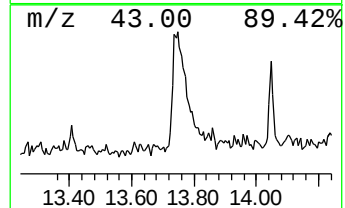
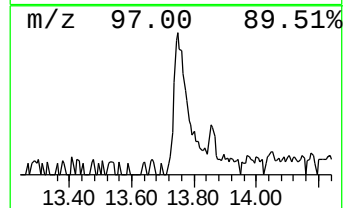
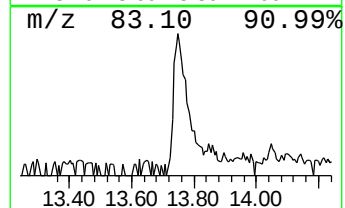
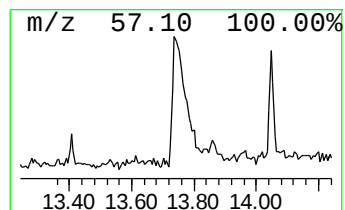
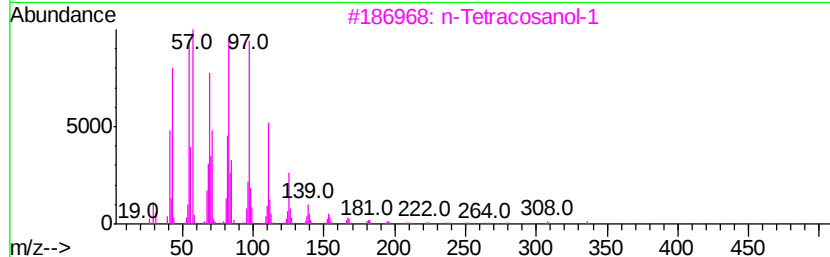
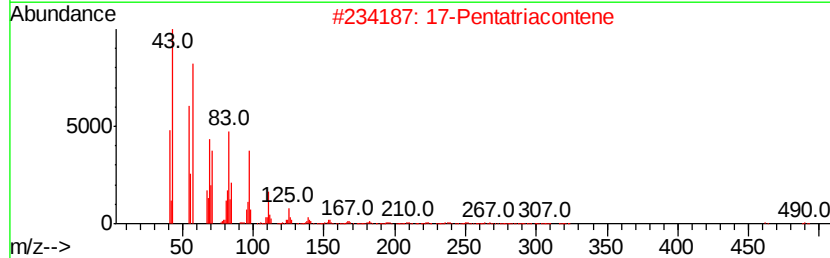
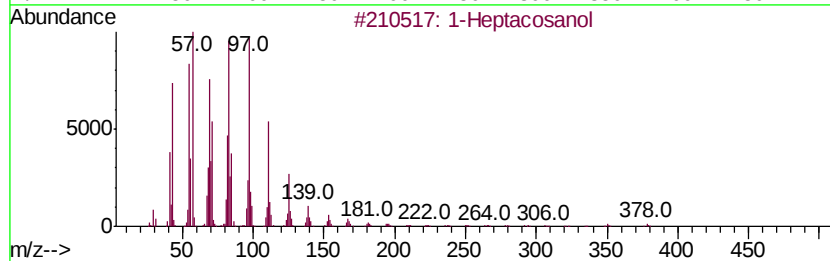
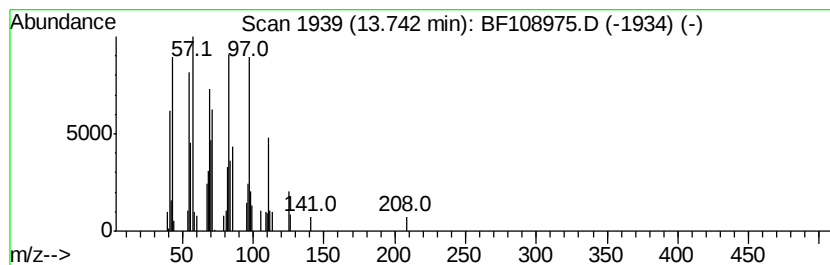
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Peak Number 4 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	3.40 ng	155984	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5		1-Hexacosanol	382	C26H54O	000506-52-5	90



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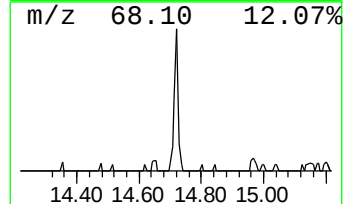
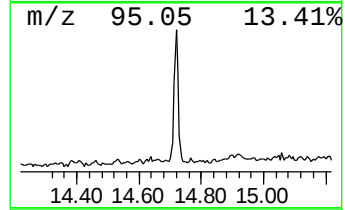
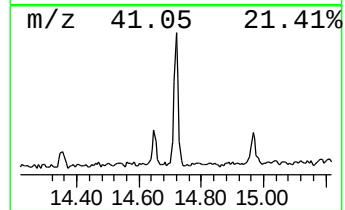
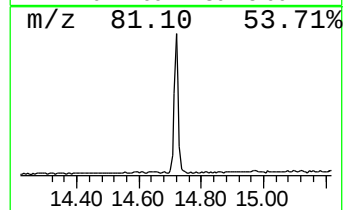
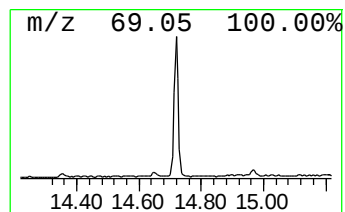
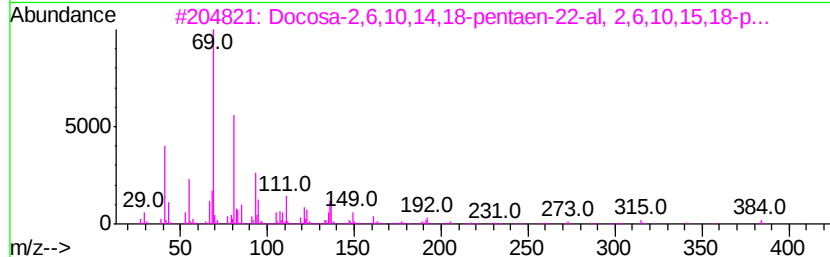
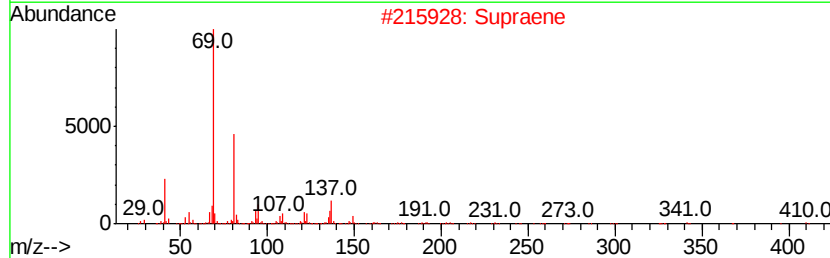
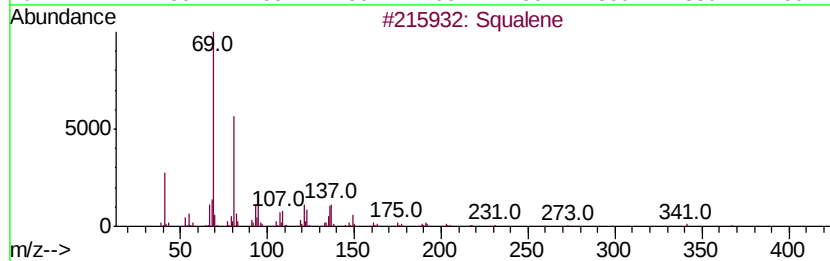
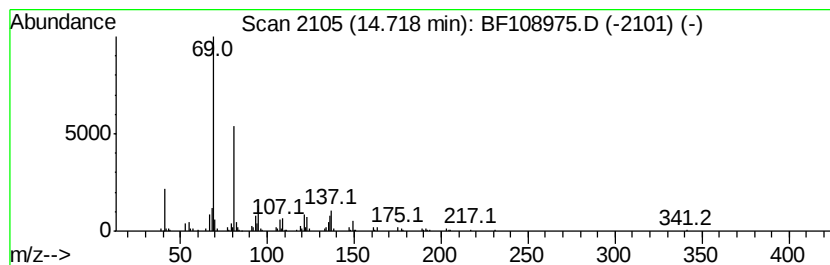
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Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	4.04 ng	202423	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4		2,7,11-Trimethyl-4-phenylthiodod...	314	C21H30S	1000190-11-3	78
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72



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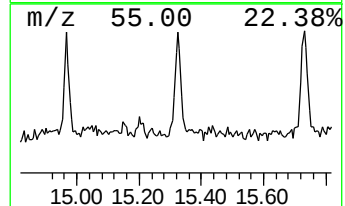
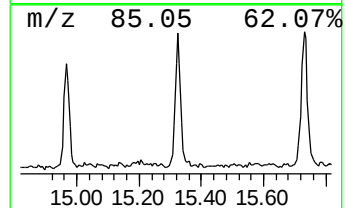
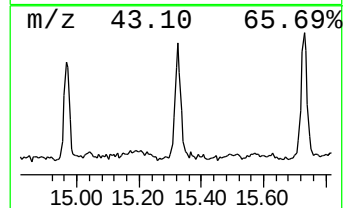
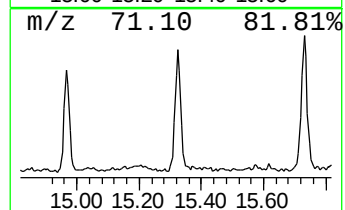
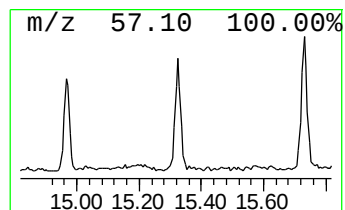
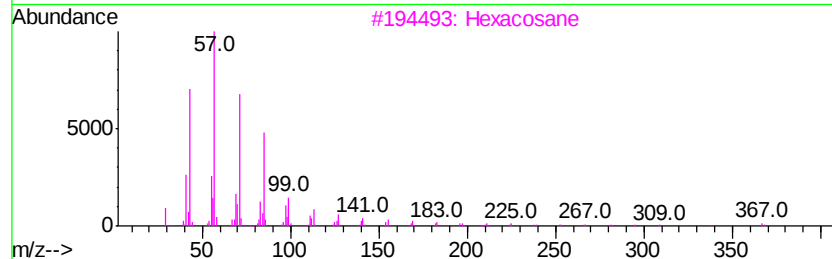
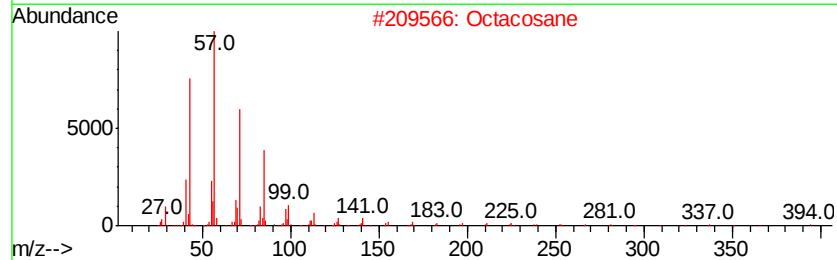
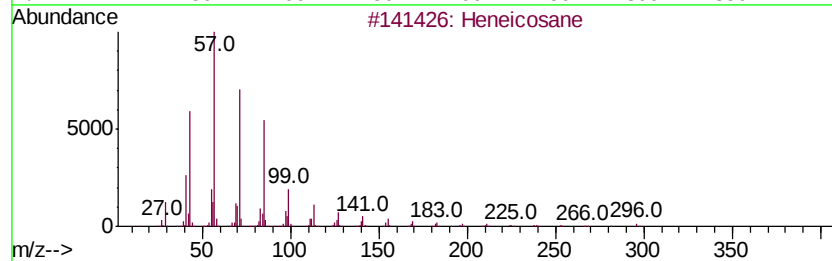
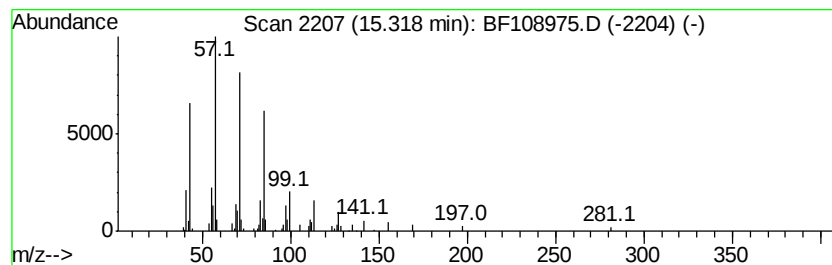
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	2.38 ng	119374	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octacosane		394	C28H58	000630-02-4	91
3	Hexacosane		366	C26H54	000630-01-3	91
4	triacontane		422	C30H62	000638-68-6	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.91	2.9	ng	116696	1	6.73	798838	20.0
unknown6.50	6.50	55.4	ng	2214100	1	6.73	798838	20.0
1-Heptacosanol	13.74	3.4	ng	155984	5	13.86	917523	20.0
Squalene	14.72	4.0	ng	202423	6	15.27	1001460	20.0
Heneicosane	15.32	2.4	ng	119374	6	15.27	1001460	20.0