

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
 Data File : BF123936.D
 Acq On : 15 May 2021 9:36
 Operator : JU/CG
 Sample : PB136395BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136395BL

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123936.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.275	26	32	38	rVB	46250	65355	2.95%	0.513%
2	2.387	46	51	55	rVB	42163	51574	2.33%	0.405%
3	5.522	579	584	587	rBV	1508678	1663243	74.99%	13.068%
4	6.522	747	754	756	rBV	1377645	1636263	73.78%	12.856%
5	6.898	815	818	822	rBV	375899	306363	13.81%	2.407%
6	7.463	908	914	917	rBV	986290	1097061	49.46%	8.619%
7	8.181	1032	1036	1039	rBV	426169	397134	17.91%	3.120%
8	9.263	1214	1220	1223	rBV	2157391	1995711	89.98%	15.680%
9	9.939	1330	1335	1338	rBV	581743	458579	20.68%	3.603%
10	10.727	1462	1469	1472	rBV	1567498	1357913	61.23%	10.669%
11	11.422	1583	1587	1591	rBV	515738	466307	21.02%	3.664%
12	11.933	1671	1674	1680	rBV3	28662	38757	1.75%	0.305%
13	12.727	1805	1809	1815	rBV3	28746	42300	1.91%	0.332%
14	13.016	1853	1858	1861	rBV	2434495	2217878	100.00%	17.426%
15	13.221	1886	1893	1901	rBV5	14469	39919	1.80%	0.314%
16	14.063	2029	2036	2040	rVB	475982	414674	18.70%	3.258%
17	14.186	2050	2057	2063	rBV5	14245	30124	1.36%	0.237%
18	14.927	2173	2183	2184	rBV7	17658	35847	1.62%	0.282%
19	15.551	2283	2289	2294	rBV2	286947	348450	15.71%	2.738%
20	16.051	2368	2374	2380	rVB3	17674	28570	1.29%	0.224%
21	16.580	2457	2464	2472	rBV4	19461	35746	1.61%	0.281%

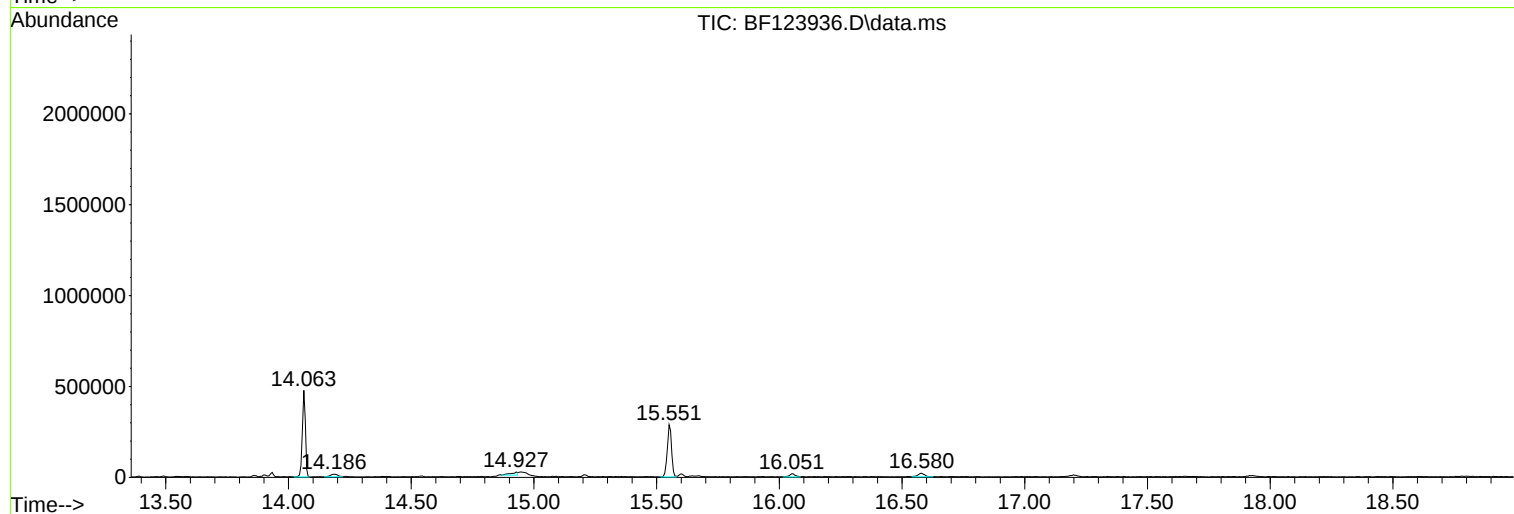
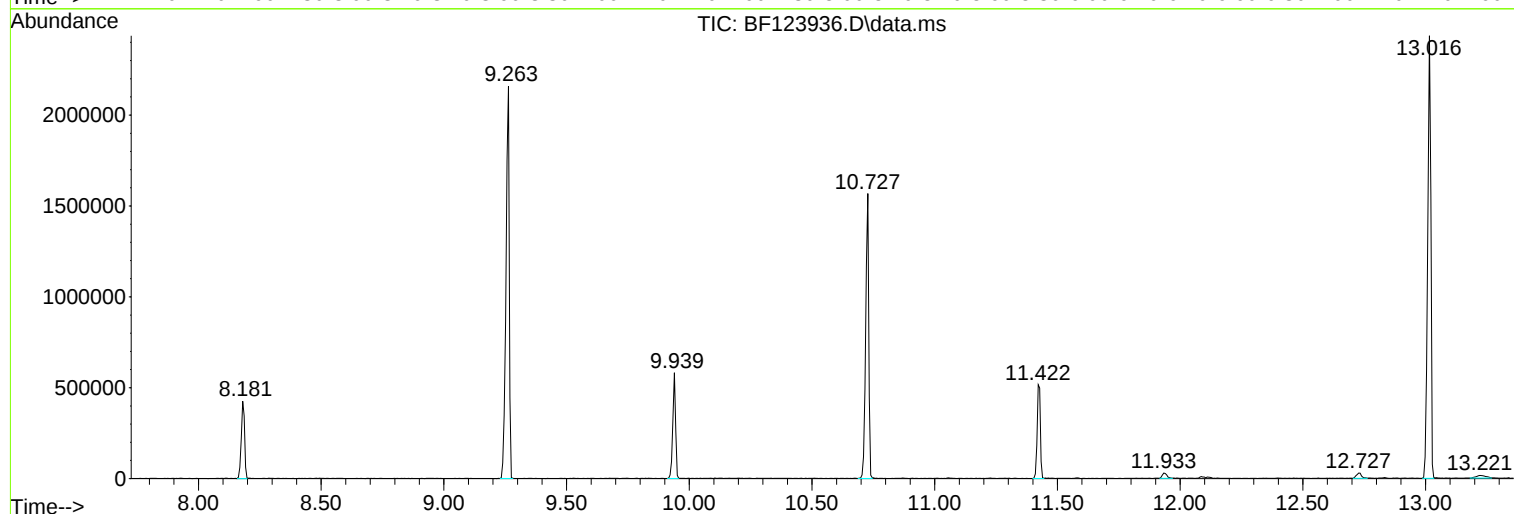
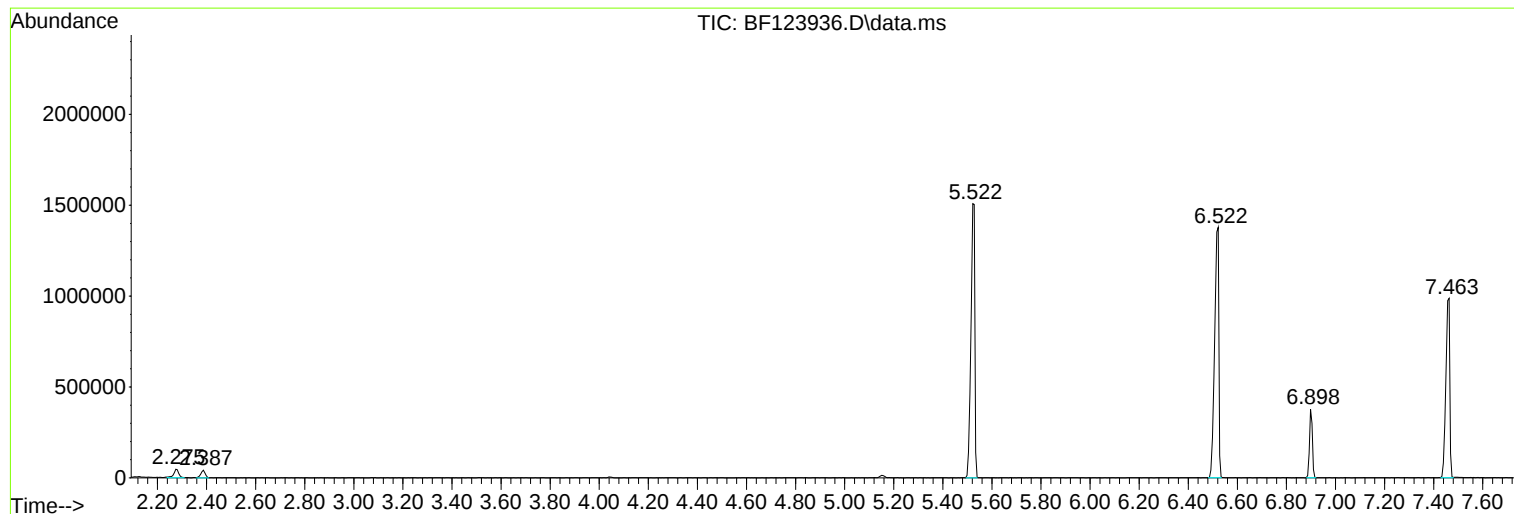
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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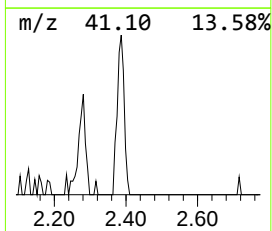
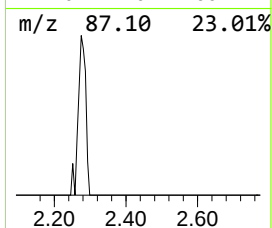
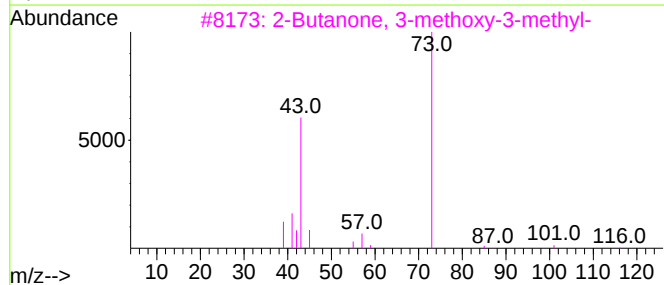
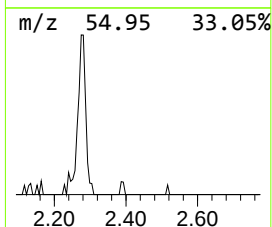
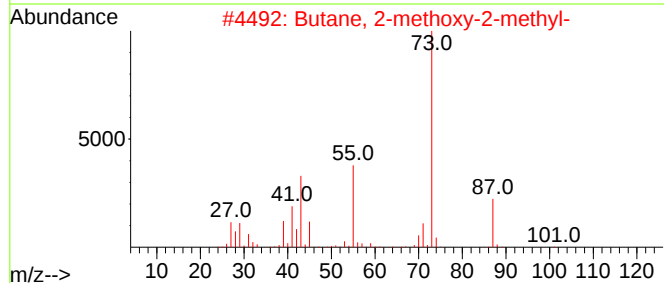
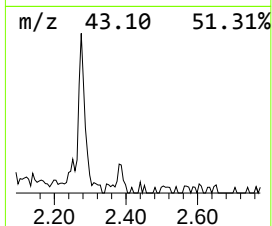
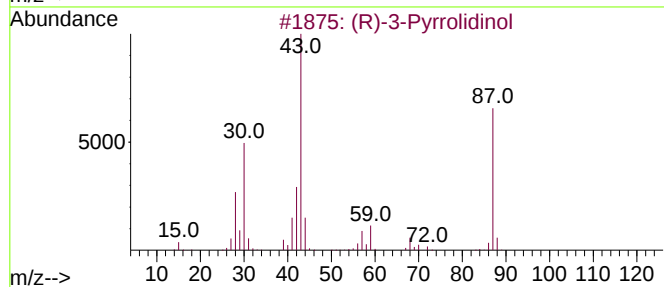
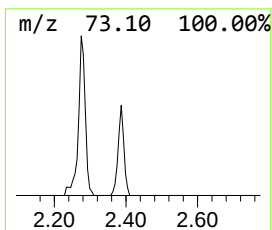
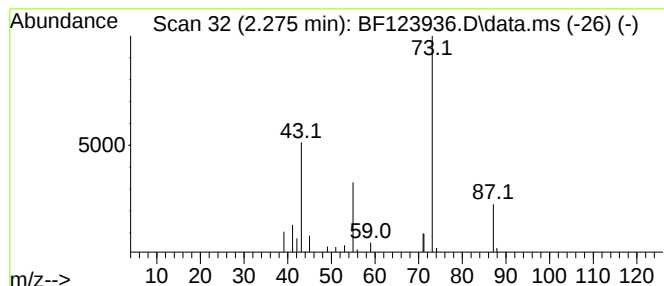
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.275 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.275	4.27 ng	65355	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-3-Pyrrolidinol			87	C4H9NO	002799-21-5	9
2	Butane, 2-methoxy-2-methyl-			102	C6H14O	000994-05-8	9
3	2-Butanone, 3-methoxy-3-methyl-			116	C6H12O2	036687-98-6	9
4	2-Methyl-5-hexen-3-ol			114	C7H14O	032815-70-6	9
5	Propanoic acid, 2-methyl-			88	C4H8O2	000079-31-2	7



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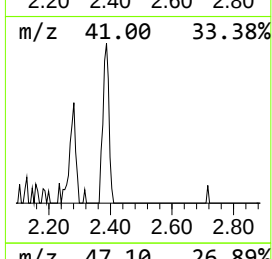
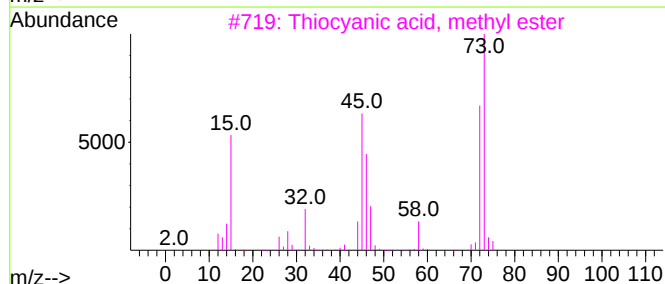
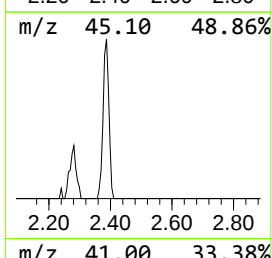
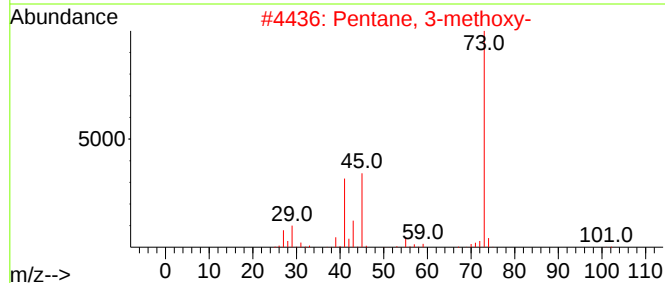
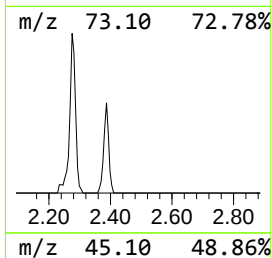
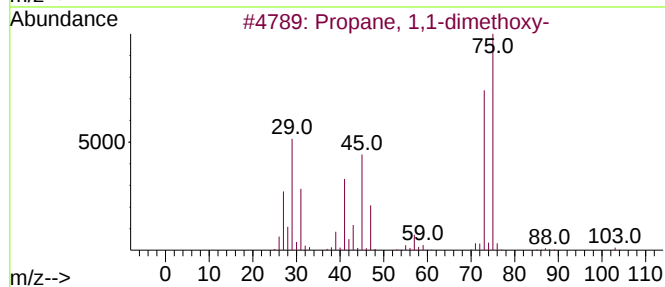
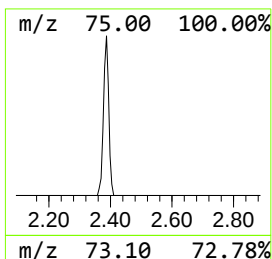
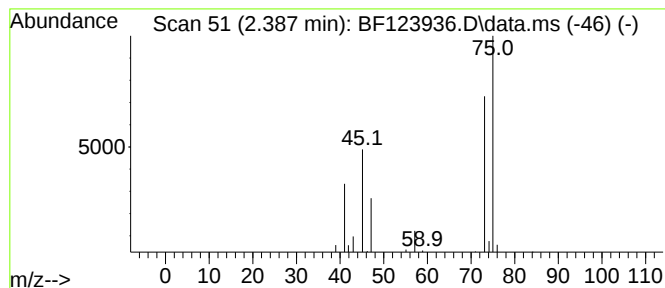
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.387	3.37 ng	51574	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
3			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
4			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	9
5			1,2,4-Butanetriol	106	C4H10O3	003068-00-6	9



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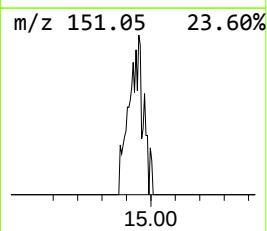
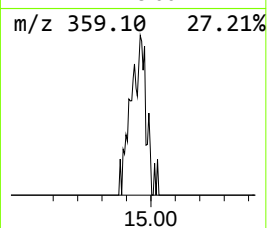
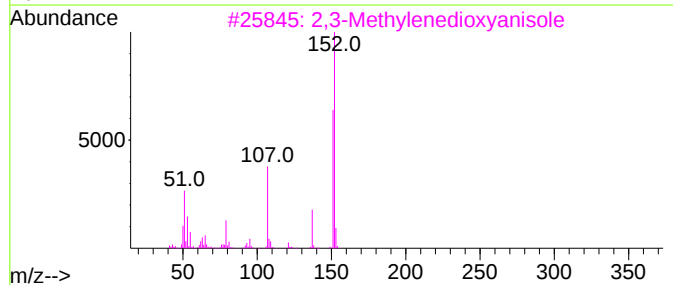
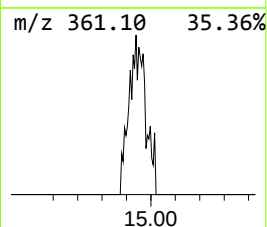
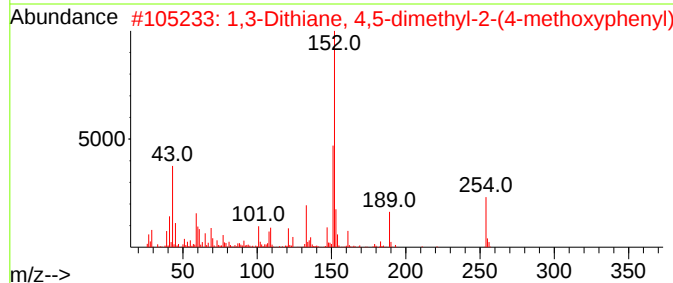
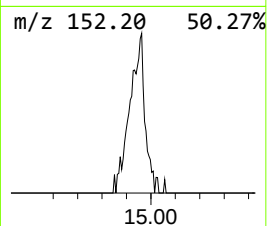
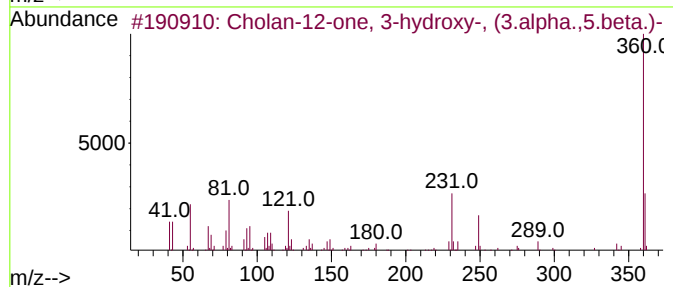
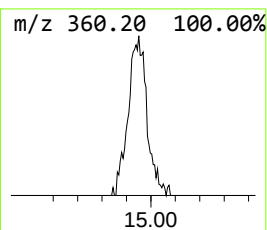
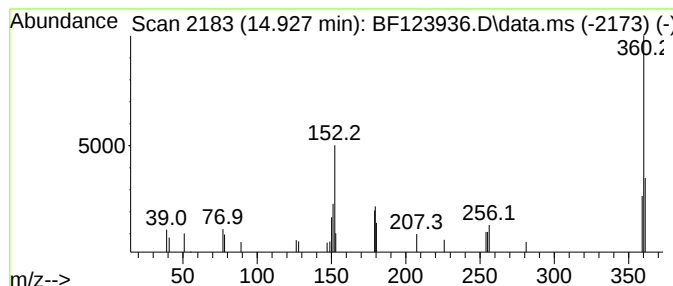
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Peak Number 3 unknown14.927 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	2.06 ng	35847	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholan-12-one, 3-hydroxy-, (3.alpha...	360	C24H40O2	054411-58-4	16
2			1,3-Dithiane, 4,5-dimethyl-2-(4-...	254	C13H18OS2	1000197-88-6	10
3			2,3-Methylenedioxyanisole	152	C8H8O3	001817-95-4	9
4			Piperonyl alcohol	152	C8H8O3	000495-76-1	9
5			Titanium, [(1,2,3,4-.eta.)-1,3,5...	256	C16H16Ti	012112-27-5	9



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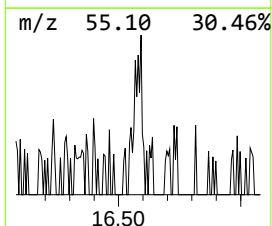
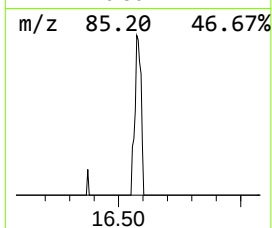
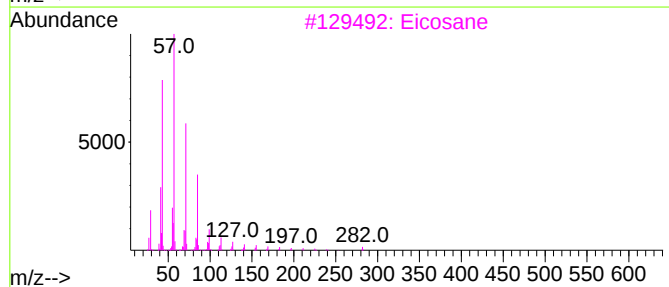
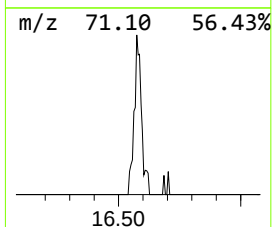
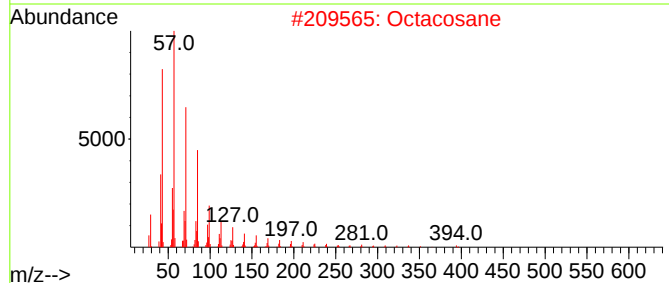
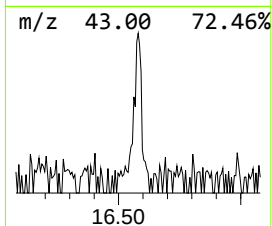
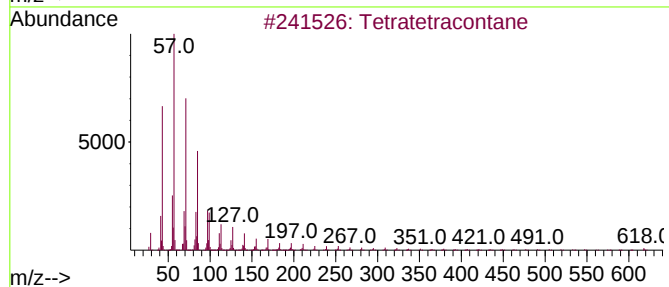
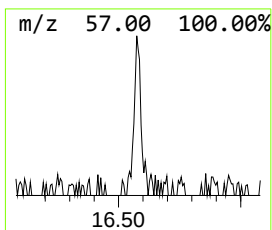
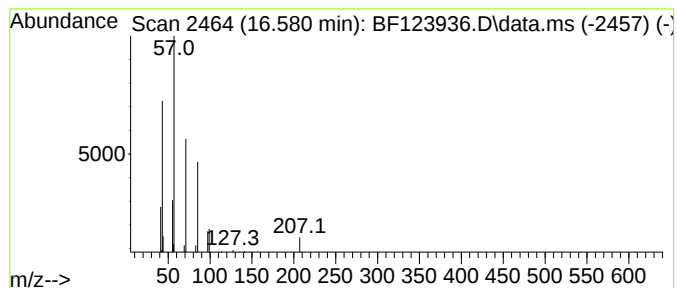
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Peak Number 4 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.580	2.05 ng	35746	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	78
2			Octacosane	394	C28H58	000630-02-4	72
3			Eicosane	282	C20H42	000112-95-8	72
4			2-Bromotetradecane	276	C14H29Br	074036-95-6	72
5			Heptadecane	240	C17H36	000629-78-7	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.275	2.275	4.3	ng	65355	1	6.898	306363	20.0
Propane, 1,1-di...	2.387	3.4	ng	51574	1	6.898	306363	20.0
unknown14.927	14.927	2.1	ng	35847	6	15.551	348450	20.0
Tetratetracontane	16.580	2.0	ng	35746	6	15.551	348450	20.0