

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011823\
 Data File : BF132135.D
 Acq On : 19 Jan 2023 00:20
 Operator : CG\JU
 Sample : 01190-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-4

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-BF011823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.349	418	427	438	rBV	1594140	2036248	37.27%	5.356%
2	5.725	485	491	494	rBV	3978382	4169343	76.31%	10.967%
3	6.707	652	658	661	rBV	3673948	4210046	77.05%	11.075%
4	7.095	720	724	727	rBV	1591595	1276792	23.37%	3.359%
5	7.654	814	819	822	rBV	2785368	2796497	51.18%	7.356%
6	8.378	938	942	946	rBV	1791592	1606283	29.40%	4.225%
7	9.460	1121	1126	1129	rBV	5109383	4831038	88.42%	12.708%
8	10.142	1239	1242	1246	rVB	2000906	1850918	33.88%	4.869%
9	10.860	1360	1364	1370	rVB	216372	161287	2.95%	0.424%
10	10.936	1373	1377	1381	rBV	3623429	3335084	61.04%	8.773%
11	11.036	1391	1394	1404	rVB2	49921	76571	1.40%	0.201%
12	11.642	1493	1497	1501	rBV	2252080	2016571	36.91%	5.305%
13	12.154	1580	1584	1590	rBV	289570	264367	4.84%	0.695%
14	12.942	1715	1718	1722	rBV	81485	71796	1.31%	0.189%
15	13.242	1764	1769	1772	rBV	5682798	5463770	100.00%	14.372%
16	13.436	1797	1802	1804	rBV	61500	68462	1.25%	0.180%
17	14.136	1918	1921	1922	rBV2	80856	75481	1.38%	0.199%
18	14.166	1922	1926	1946	rVV7	82279	362162	6.63%	0.953%
19	14.307	1946	1950	1954	rVV	1826764	1585328	29.02%	4.170%
20	14.395	1959	1965	1972	rVV	400925	444958	8.14%	1.170%
21	14.454	1972	1975	1979	rVB	60364	56123	1.03%	0.148%
22	15.907	2216	2222	2230	rBV	946850	1256457	23.00%	3.305%

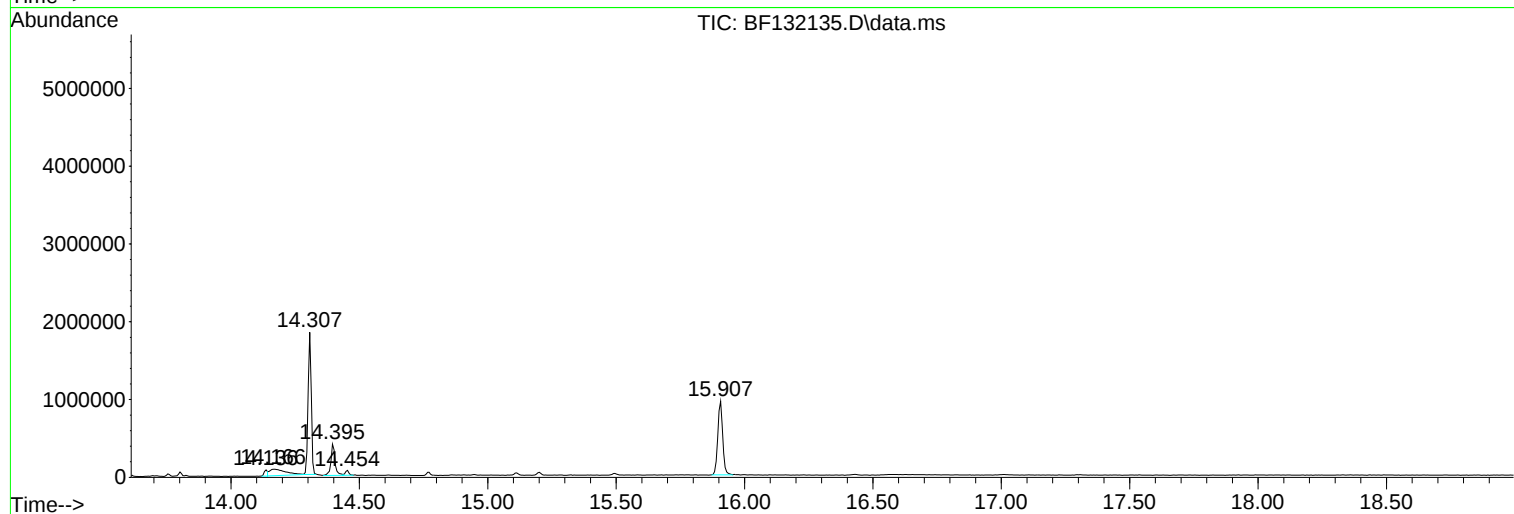
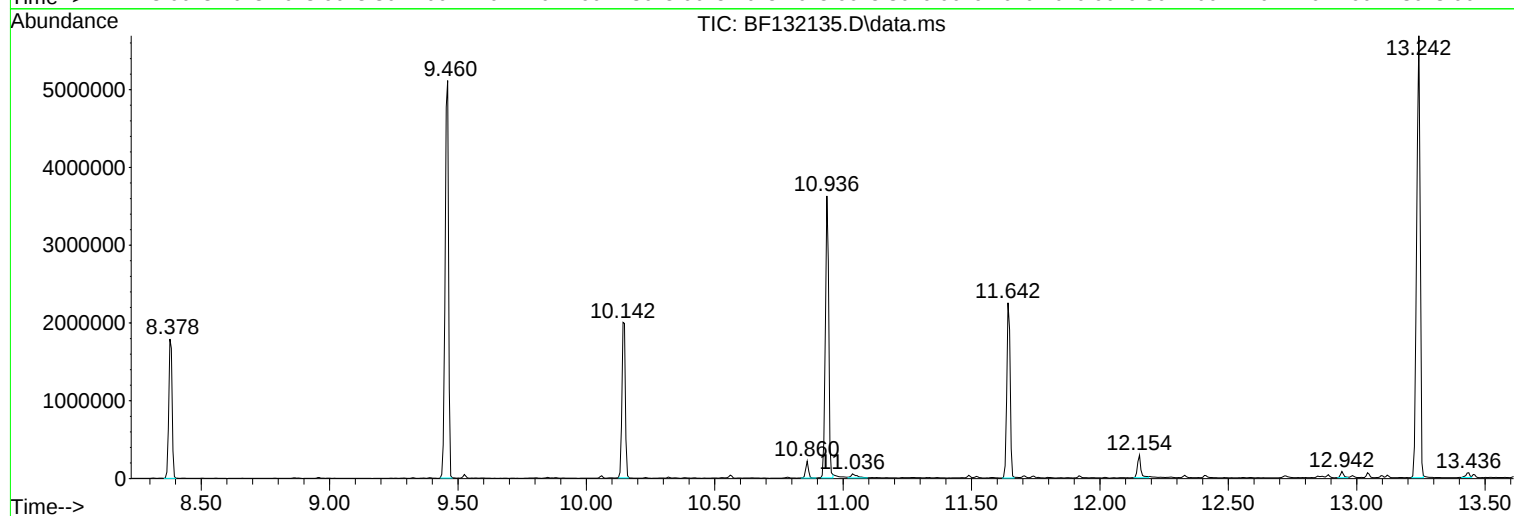
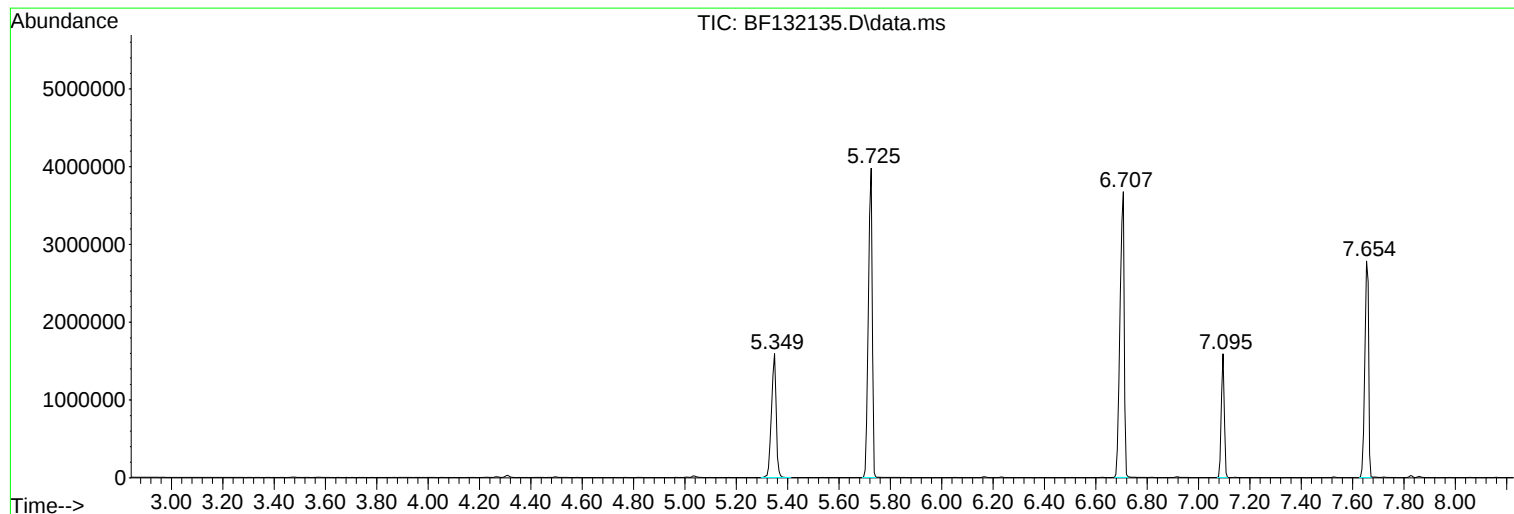
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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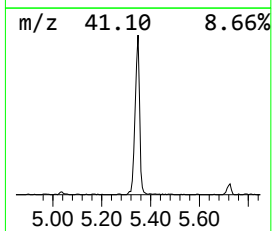
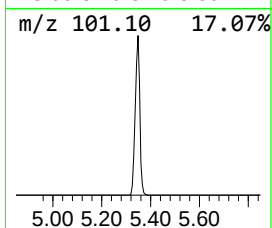
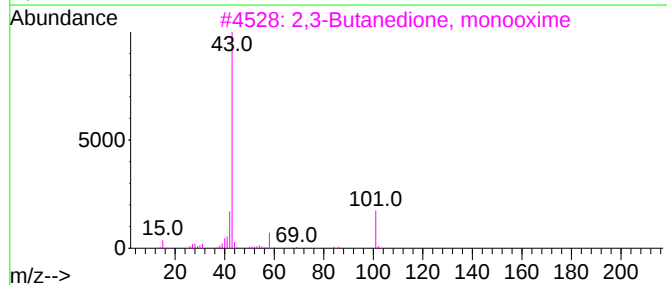
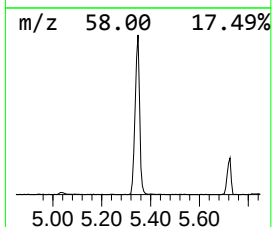
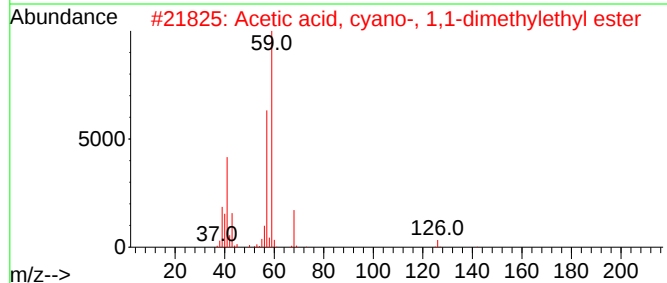
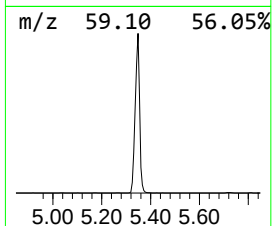
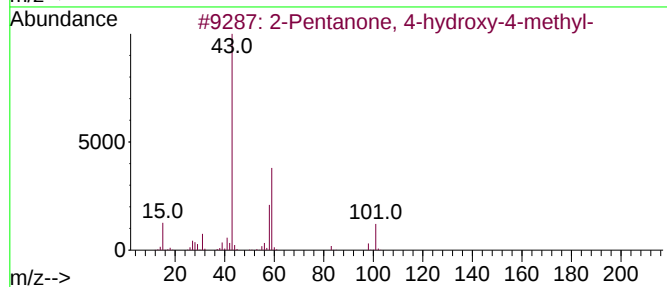
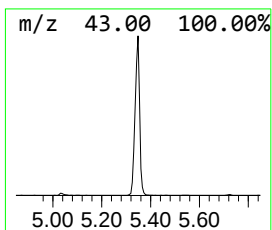
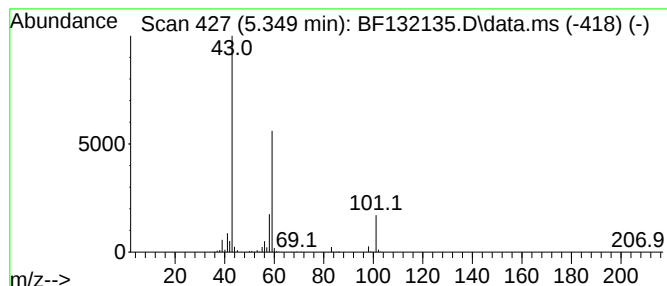
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.349	31.90 ng	2036250	1,4-Dichlorobenzene-d4	7.095

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Acetone	58	C3H6O	000067-64-1	12



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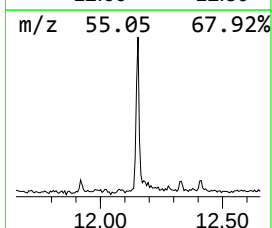
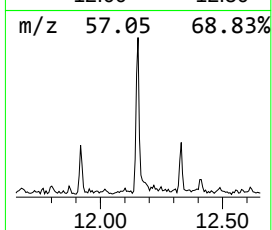
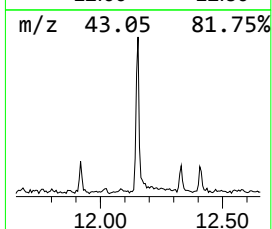
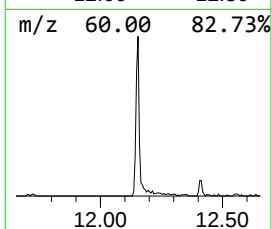
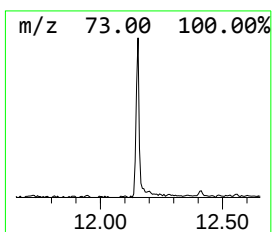
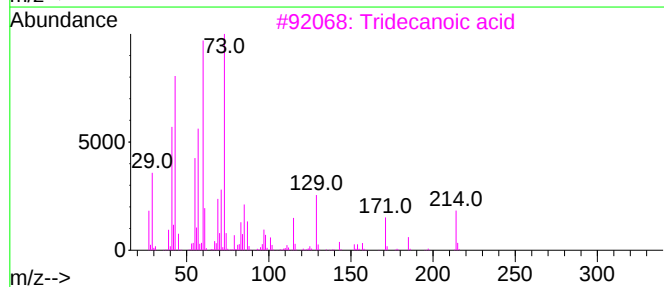
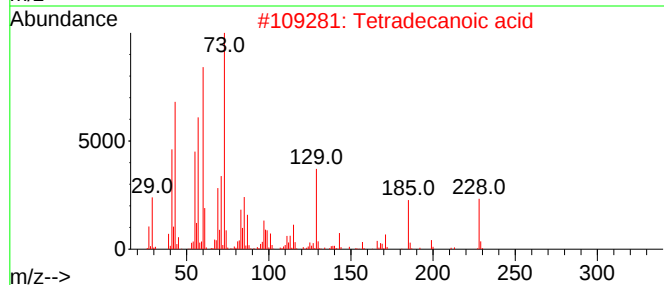
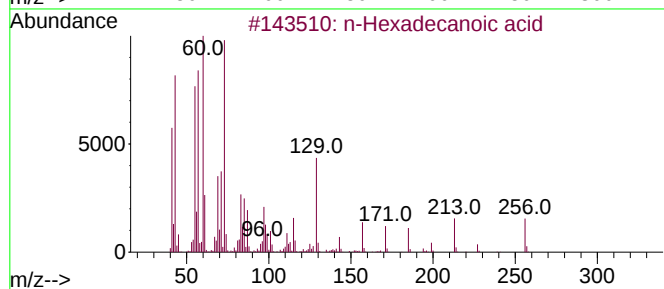
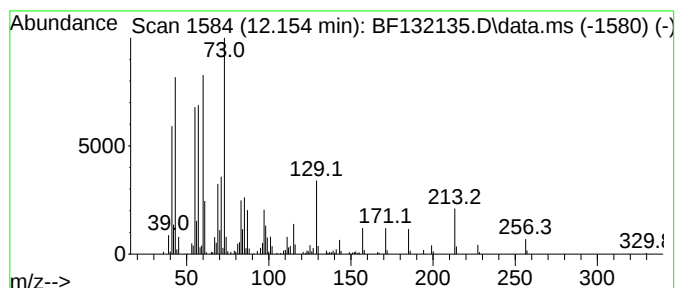
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.154	2.62 ng	264367	Phenanthrene-d10	11.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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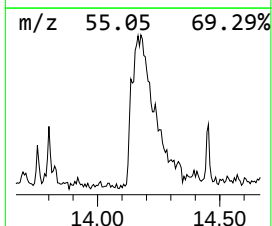
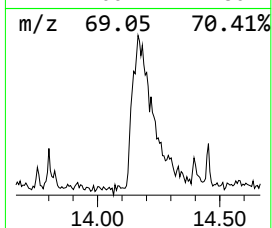
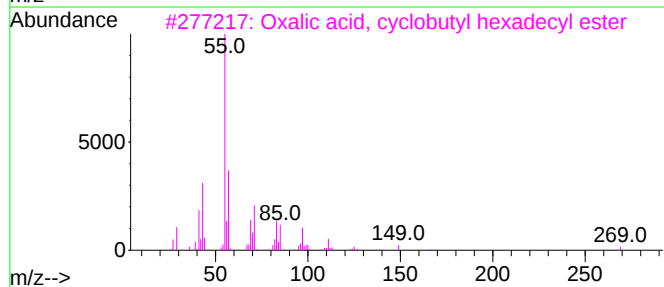
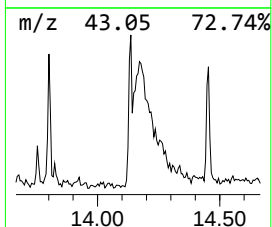
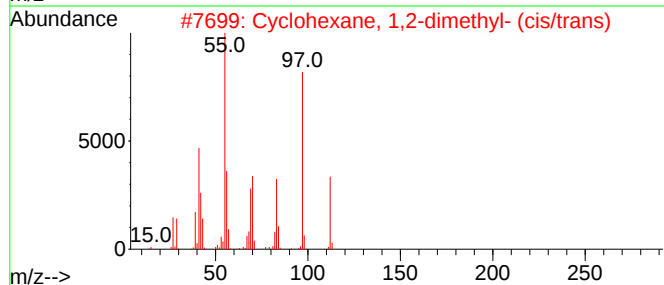
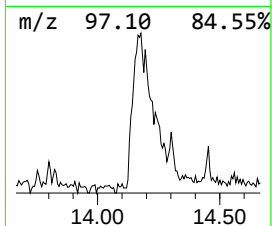
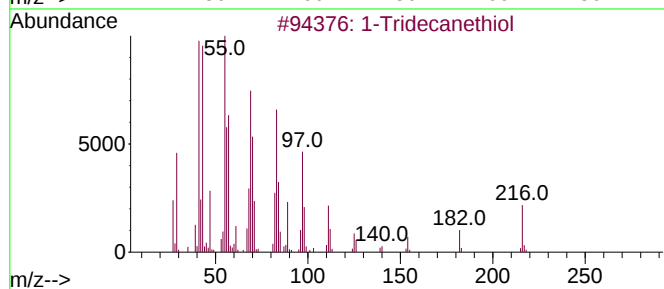
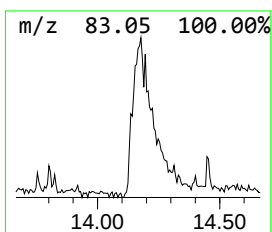
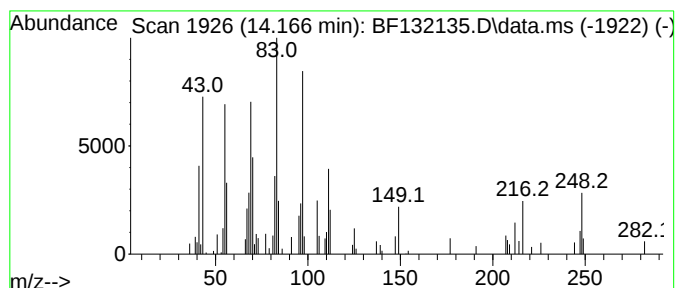
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Peak Number 3 1-Tridecanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.166	4.57 ng	362162	Chrysene-d12	14.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tridecanethiol	216	C13H28S	019484-26-5	64
2			Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	35
3			Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	35
4			Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	25
5			Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	25



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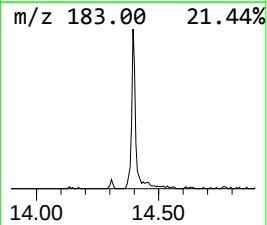
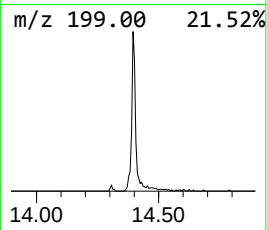
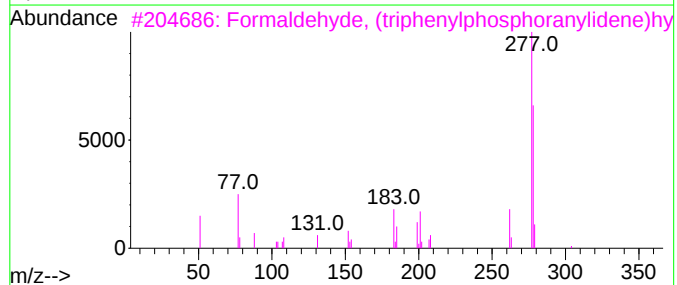
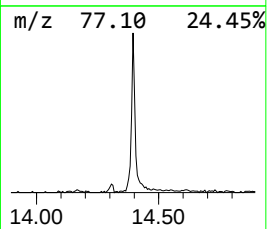
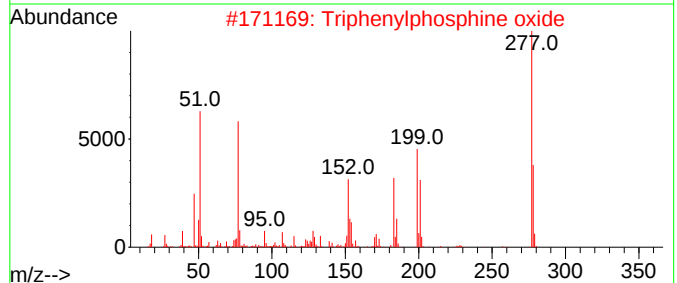
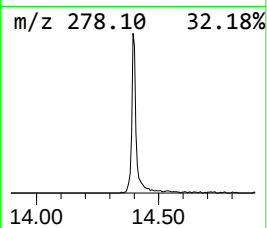
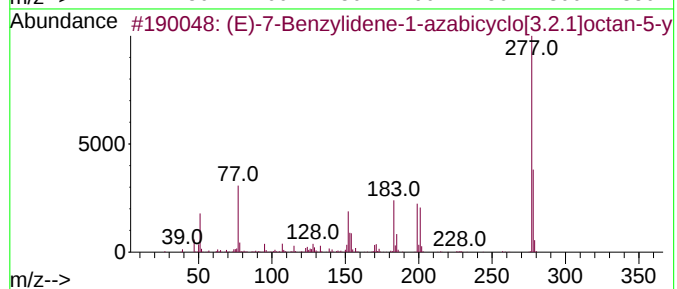
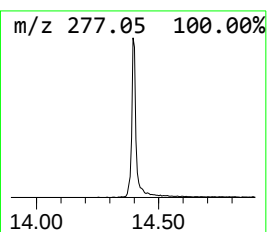
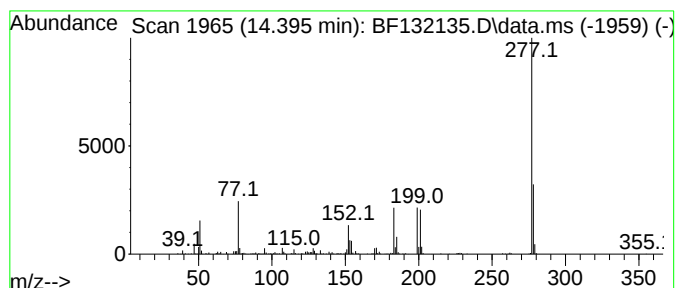
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Peak Number 4 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.395	5.61 ng	444958	Chrysene-d12	14.307

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	95		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	83		
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64		
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	37		
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.349	31.9	ng	2036250	1	7.095	1276790	20.0
n-Hexadecanoic ...	12.154	2.6	ng	264367	4	11.642	2016570	20.0
1-Tridecanethiol	14.166	4.6	ng	362162	5	14.307	1585330	20.0
(E)-7-Benzylide...	14.395	5.6	ng	444958	5	14.307	1585330	20.0