

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021623\
 Data File : BF132442.D
 Acq On : 16 Feb 2023 19:53
 Operator : CG\JU
 Sample : 01553-06
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-06

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-BF021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132442.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.319	74	82	91	rBV	45221	78806	1.07%	0.197%
2	3.684	142	144	162	rBV2	71370	136460	1.86%	0.342%
3	5.266	409	413	422	rVB	1129525	1263505	17.18%	3.163%
4	5.654	474	479	482	rBV	3598532	3285092	44.66%	8.225%
5	6.642	643	647	650	rBV	2514985	2138918	29.08%	5.355%
6	7.031	709	713	716	rBV	1231112	1102762	14.99%	2.761%
7	7.595	803	809	812	rBV	4184560	4140236	56.29%	10.366%
8	8.313	927	931	934	rBV	1808996	1442239	19.61%	3.611%
9	9.395	1110	1115	1118	rBV	7181450	6664223	90.60%	16.685%
10	10.077	1227	1231	1234	rVB	2056088	1640985	22.31%	4.109%
11	10.483	1297	1300	1305	rVB	333105	283141	3.85%	0.709%
12	10.795	1348	1353	1356	rBV	124733	117003	1.59%	0.293%
13	10.872	1361	1366	1369	rBV	4506893	4514765	61.38%	11.304%
14	11.571	1481	1485	1489	rBV	2147823	1772384	24.10%	4.438%
15	12.089	1568	1573	1586	rBV4	61701	203002	2.76%	0.508%
16	13.171	1751	1757	1760	rBV	7229152	7355250	100.00%	18.415%
17	14.230	1933	1937	1941	rBV	1765579	1581371	21.50%	3.959%
18	14.318	1947	1952	1959	rBV	575993	599905	8.16%	1.502%
19	15.101	2081	2085	2090	rVB	171784	178599	2.43%	0.447%
20	15.795	2197	2203	2211	rBV	1061225	1442090	19.61%	3.611%

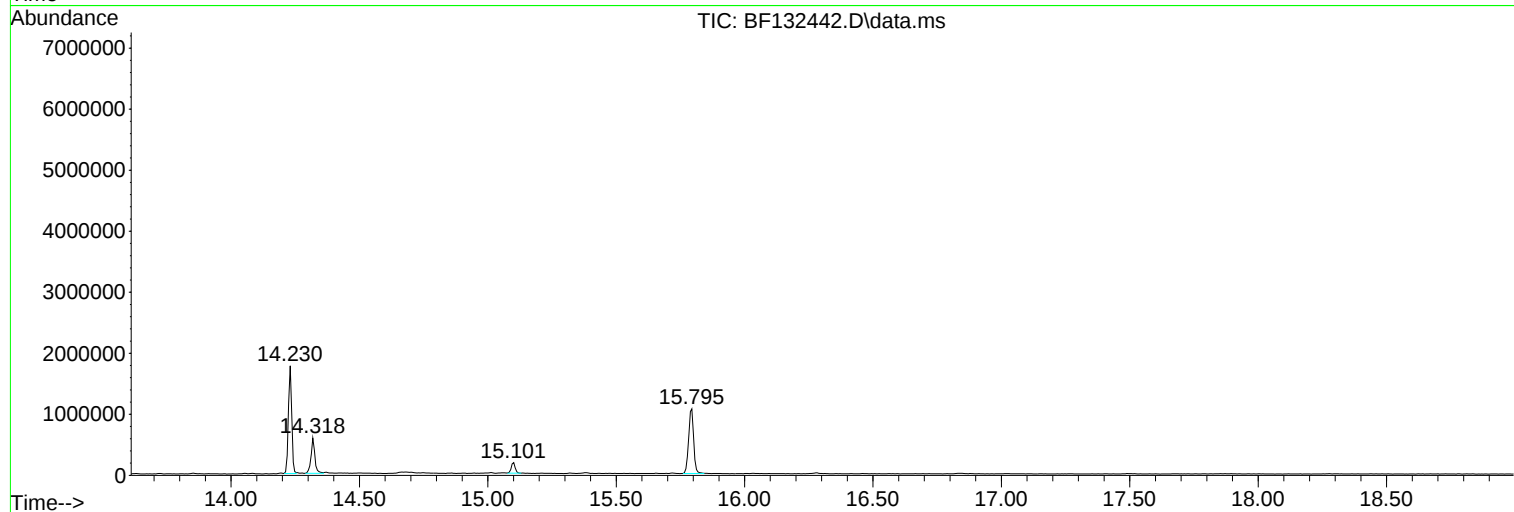
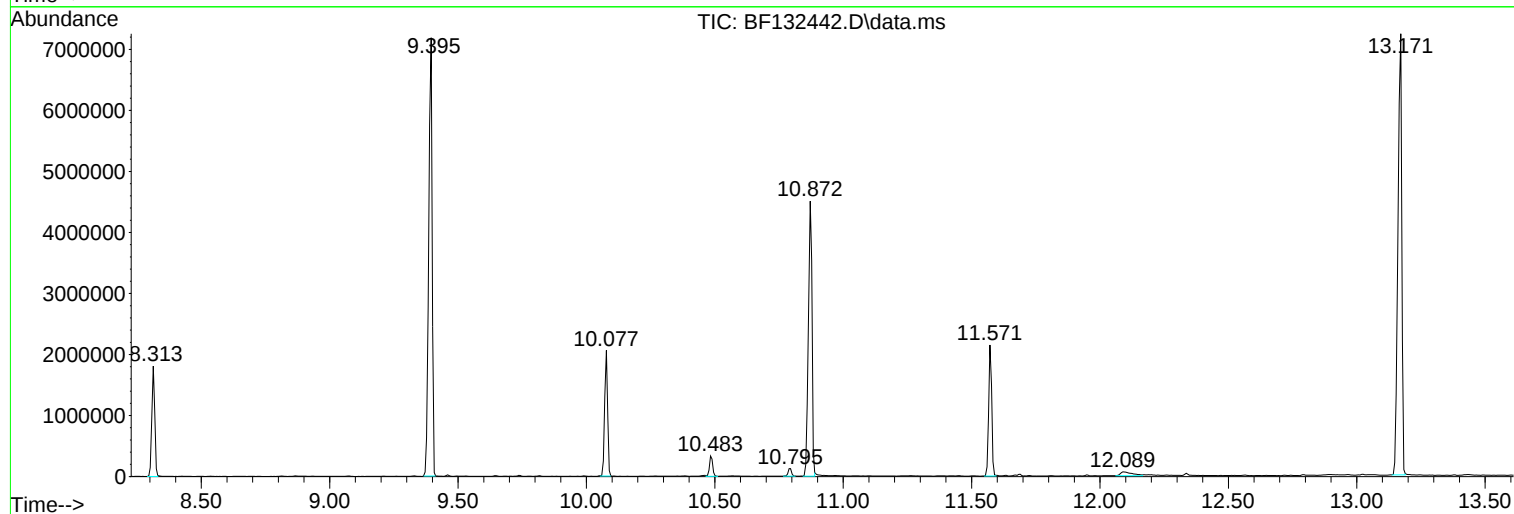
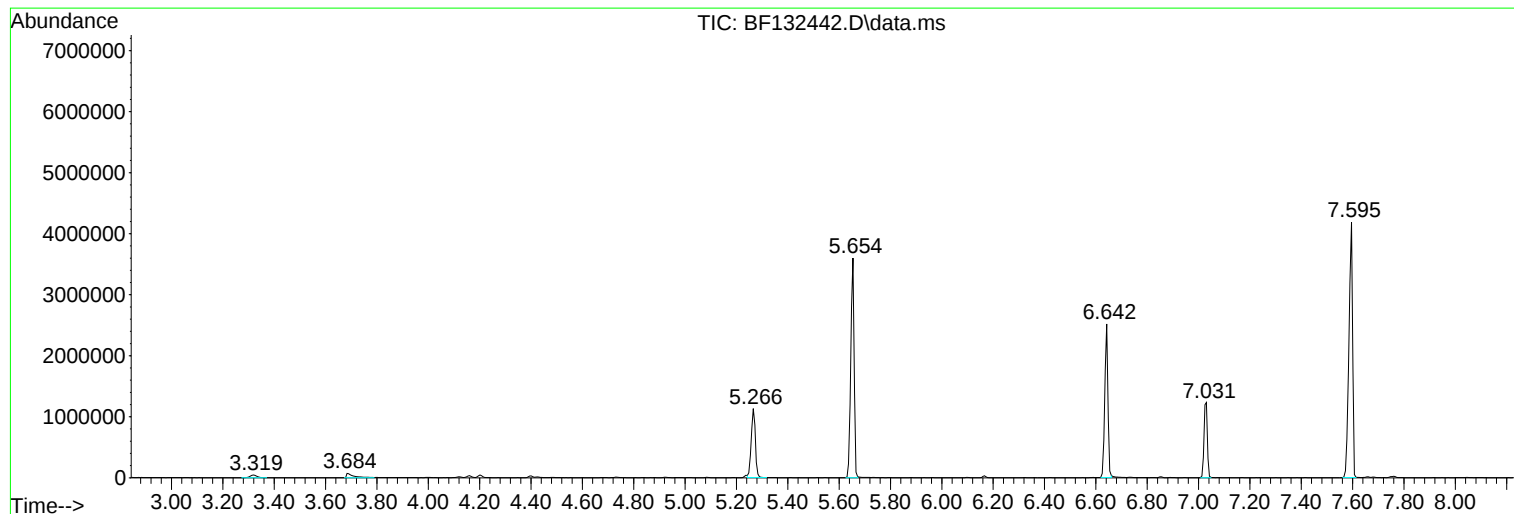
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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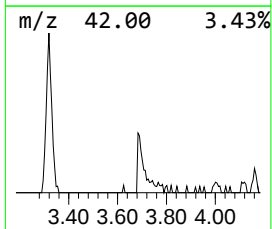
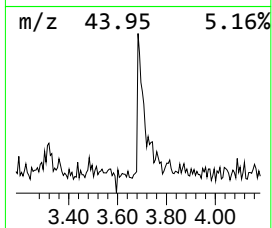
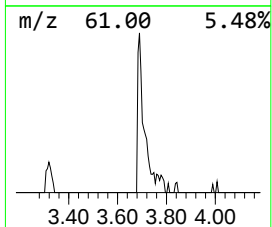
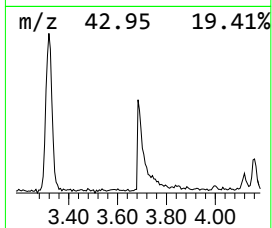
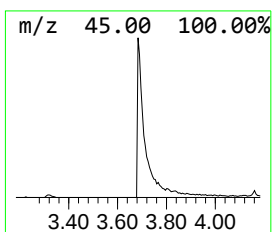
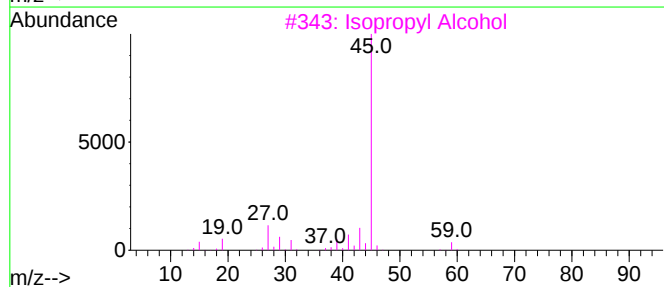
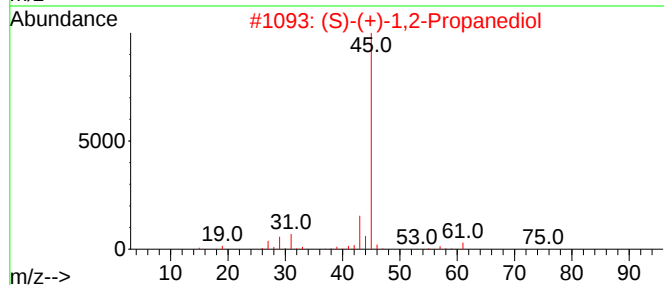
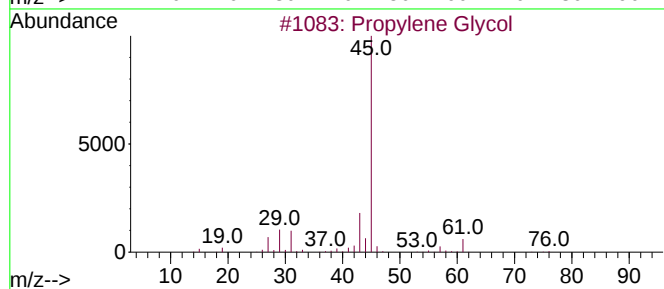
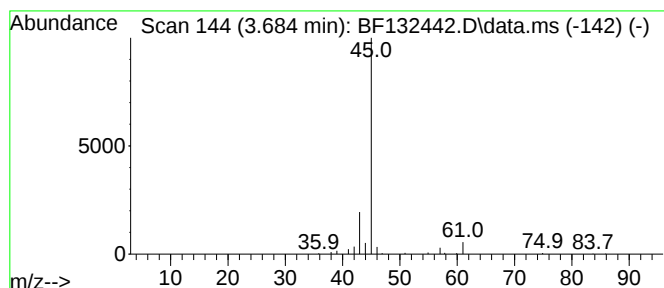
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.684 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.684	2.47 ng	136460	1,4-Dichlorobenzene-d4	7.031

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	43
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9



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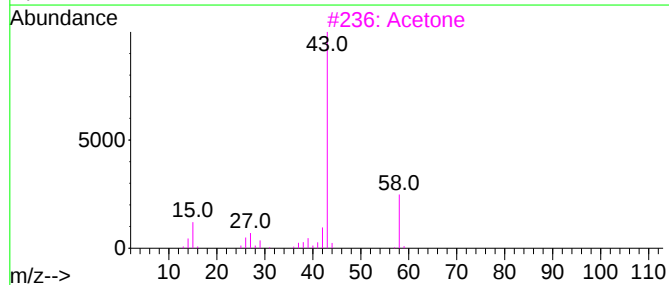
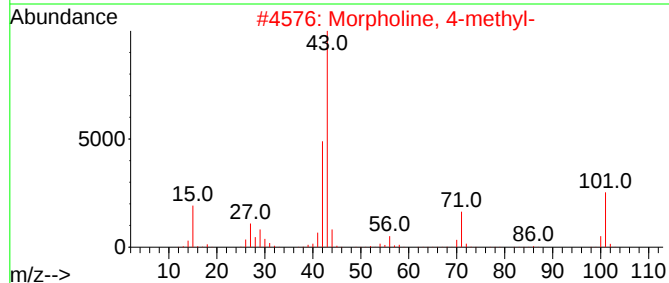
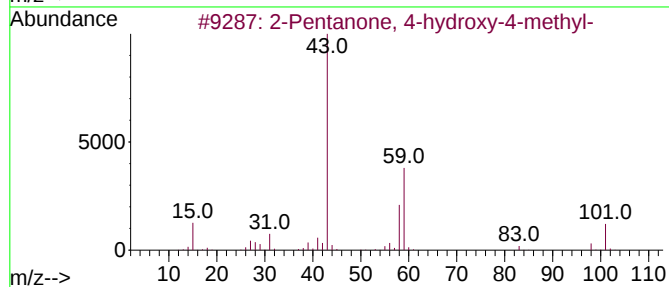
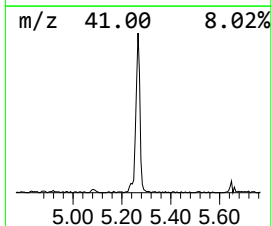
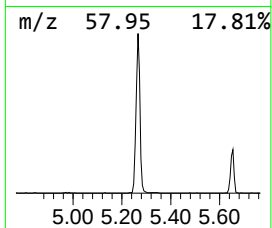
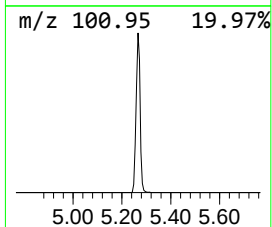
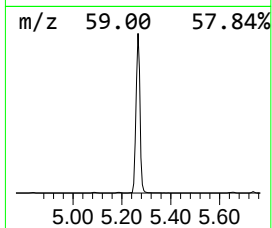
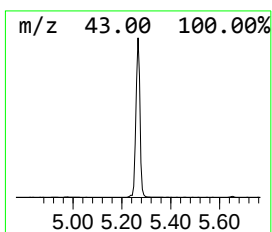
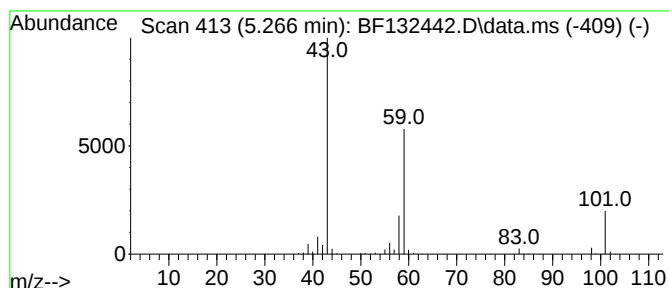
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.266	22.92 ng	1263510	1,4-Dichlorobenzene-d4	7.031

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3			Acetone	58	C3H6O	000067-64-1	9
4			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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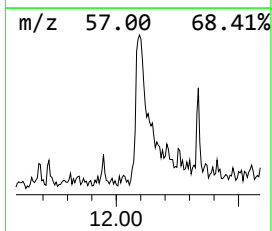
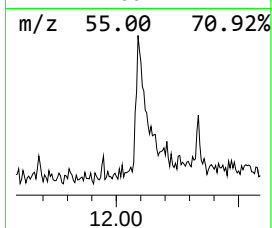
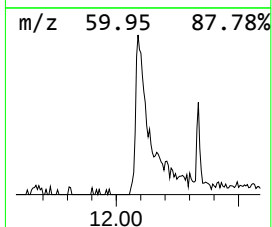
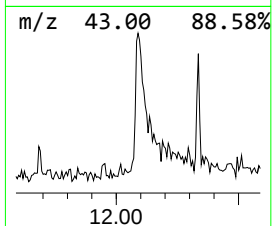
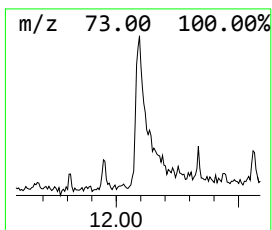
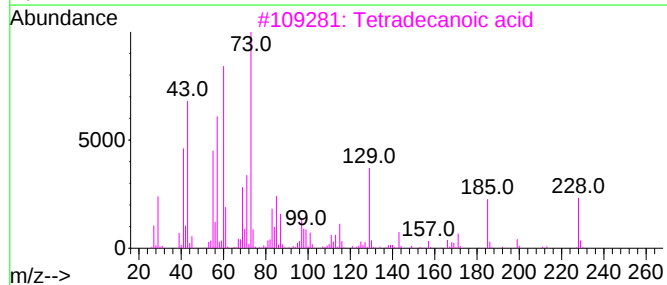
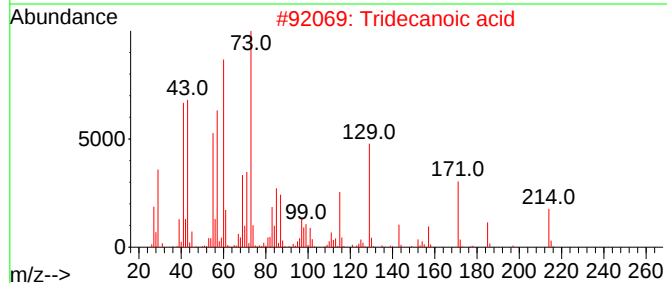
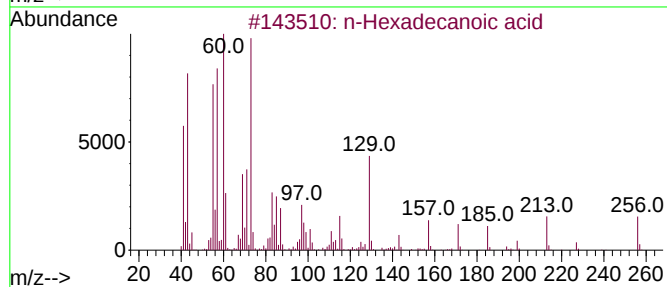
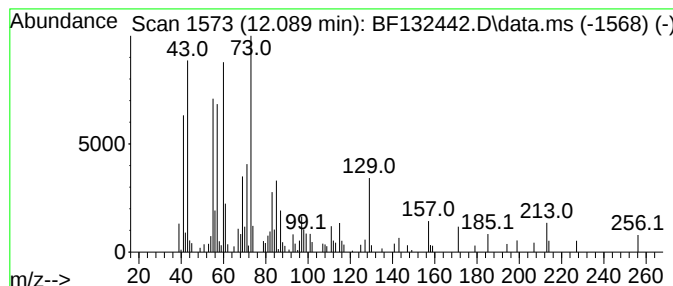
Instrument :
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.089	2.29 ng	203002	Phenanthrene-d10		11.572	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Tridecanoic acid		214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	72
5	Nonanoic acid		158	C9H18O2	000112-05-0	46



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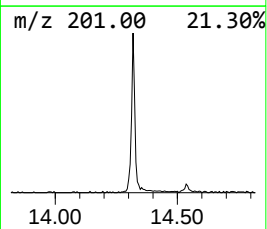
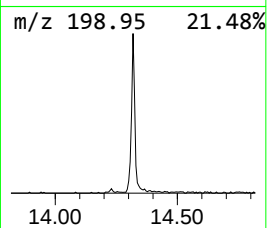
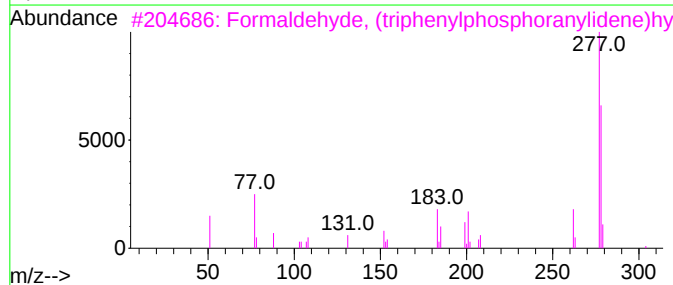
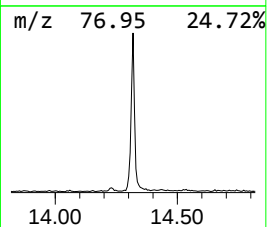
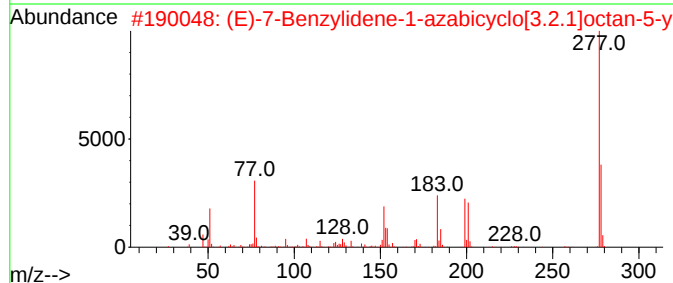
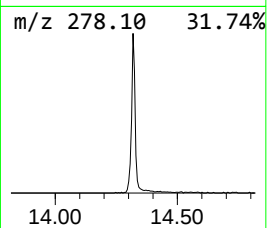
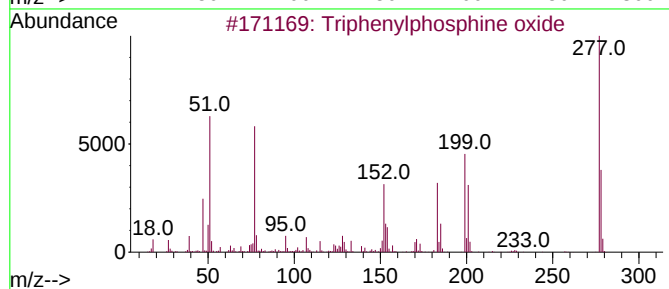
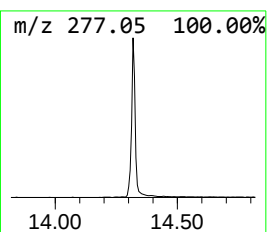
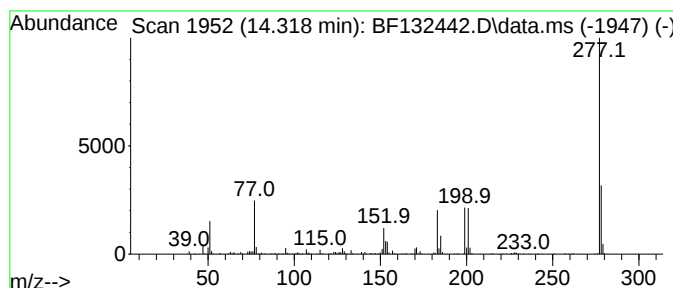
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.318	7.59 ng	599905	Chrysene-d12	14.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	92
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	87
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25



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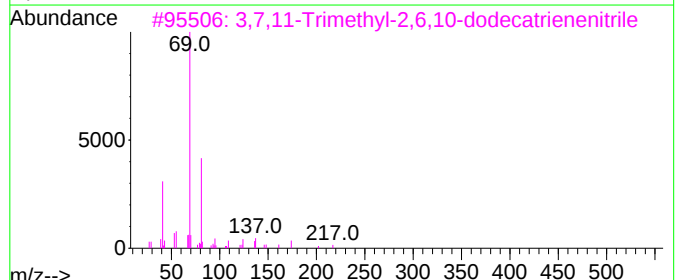
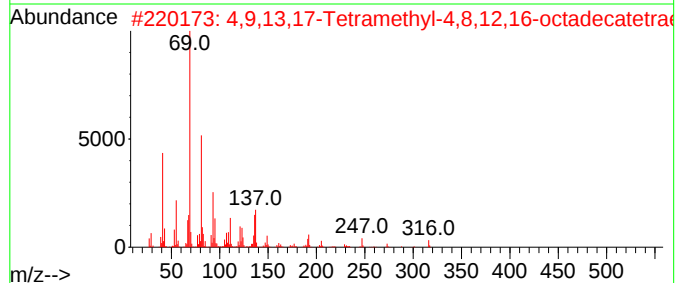
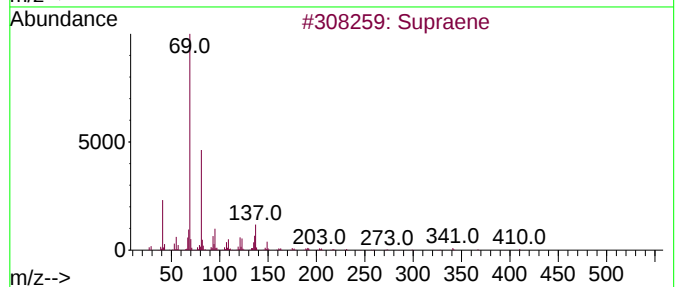
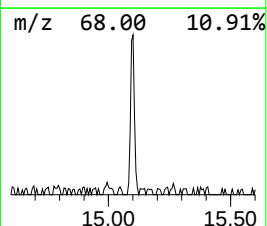
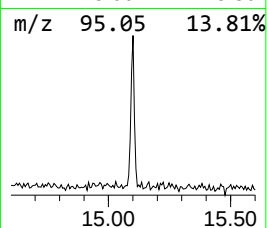
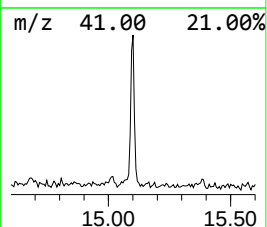
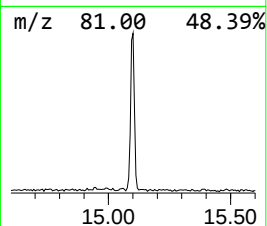
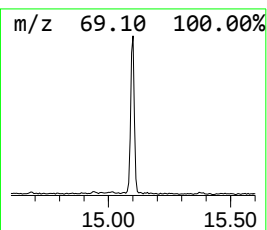
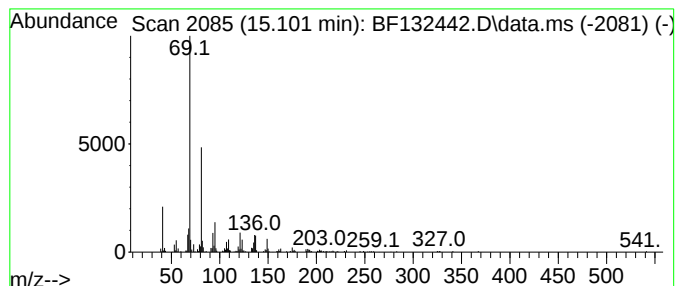
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Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.101	2.48 ng	178599	Perylene-d12	15.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
4			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	53
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.684	3.684	2.5	ng	136460	1	7.031	1102760	20.0
2-Pentanone, 4-...	5.266	22.9	ng	1263510	1	7.031	1102760	20.0
n-Hexadecanoic ...	12.089	2.3	ng	203002	4	11.572	1772380	20.0
Triphenylphosph...	14.318	7.6	ng	599905	5	14.230	1581370	20.0
Supraene	15.101	2.5	ng	178599	6	15.795	1442090	20.0