

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021323\
 Data File : BF132418.D
 Acq On : 13 Feb 2023 19:40
 Operator : CG\JU
 Sample : 01329-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-7-BORING-2-14-21

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-BF021323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132418.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.284	410	416	426	rVB	1035701	1486911	27.75%	4.190%
2	5.666	475	481	484	rBV	3311592	3666318	68.42%	10.331%
3	6.654	643	649	652	rBV	2924556	3600281	67.19%	10.145%
4	7.031	709	713	716	rBV	1084962	830568	15.50%	2.340%
5	7.601	803	810	813	rBV	2232460	2485551	46.39%	7.004%
6	8.319	928	932	935	rBV	1355936	1102689	20.58%	3.107%
7	9.395	1109	1115	1118	rBV	5290108	4994192	93.21%	14.073%
8	10.084	1228	1232	1235	rVB	1417386	1297827	24.22%	3.657%
9	10.795	1350	1353	1357	rVB	109893	85265	1.59%	0.240%
10	10.878	1362	1367	1370	rBV	4109985	3722413	69.47%	10.489%
11	11.578	1482	1486	1489	rBV	1681584	1369720	25.56%	3.860%
12	12.089	1569	1573	1588	rBV	407209	506207	9.45%	1.426%
13	12.801	1688	1694	1703	rBV6	26413	62866	1.17%	0.177%
14	12.878	1704	1707	1720	rVV2	68602	112548	2.10%	0.317%
15	13.177	1752	1758	1761	rBV	5179387	5358190	100.00%	15.098%
16	14.236	1934	1938	1942	rBV	1388336	1227997	22.92%	3.460%
17	14.324	1947	1953	1959	rBV	1019739	1084973	20.25%	3.057%
18	14.866	2041	2045	2050	rBV	473115	429161	8.01%	1.209%
19	15.107	2082	2086	2097	rVB	800343	822433	15.35%	2.317%
20	15.801	2198	2204	2211	rBV2	947955	1242311	23.19%	3.501%

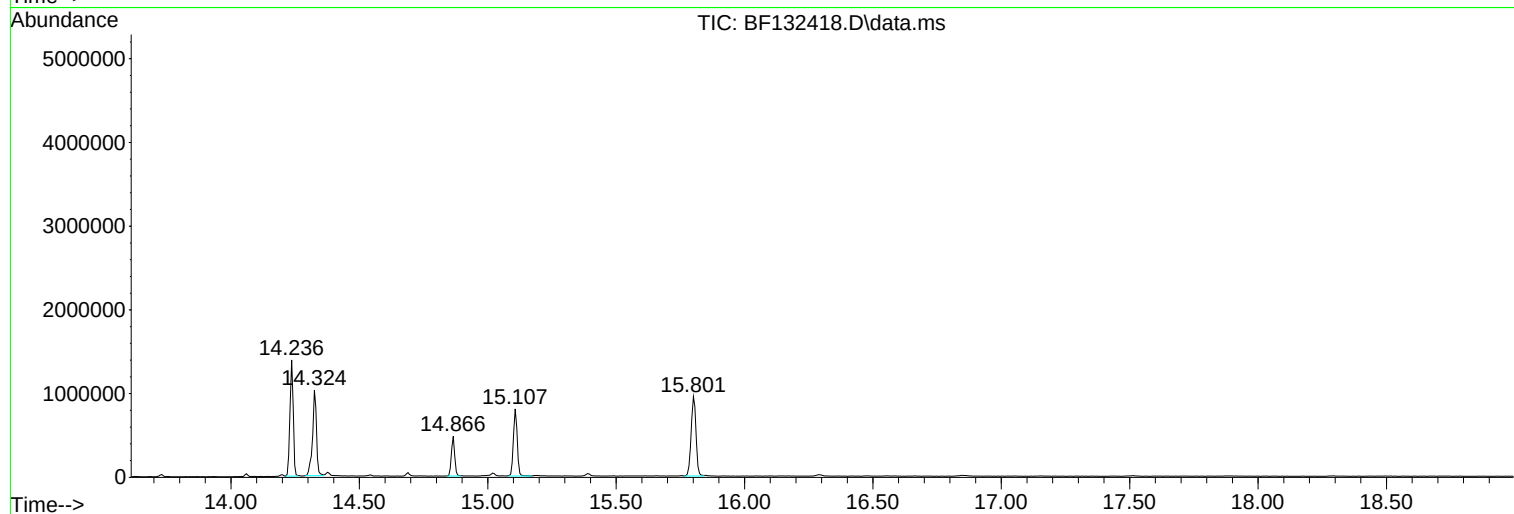
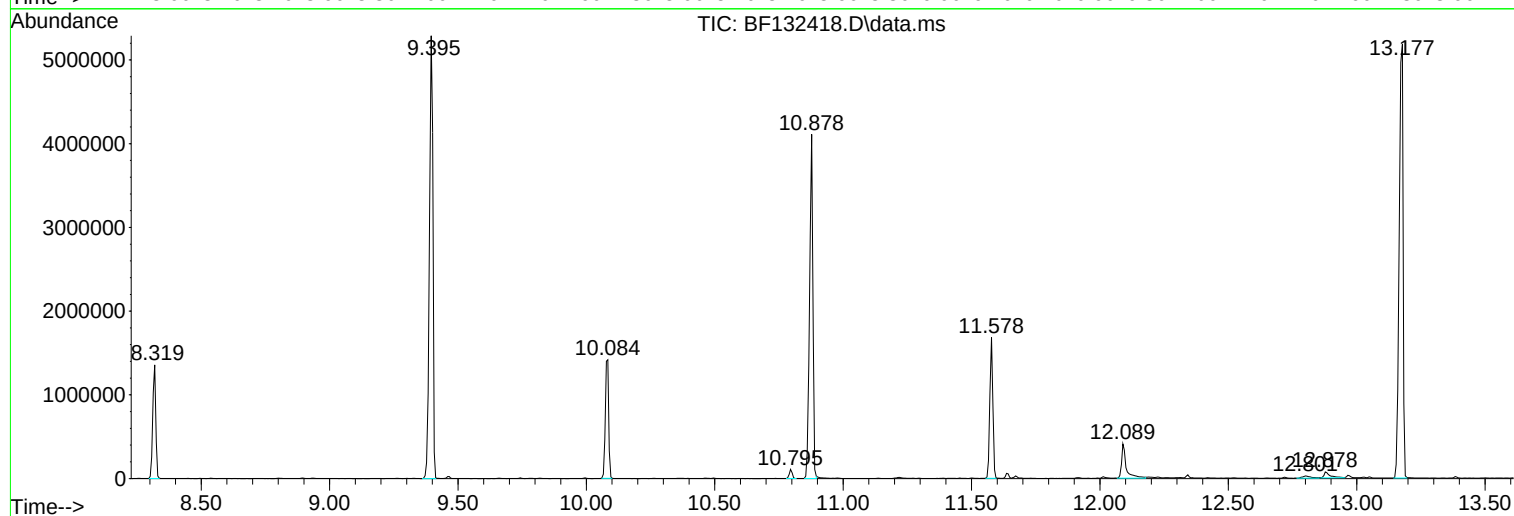
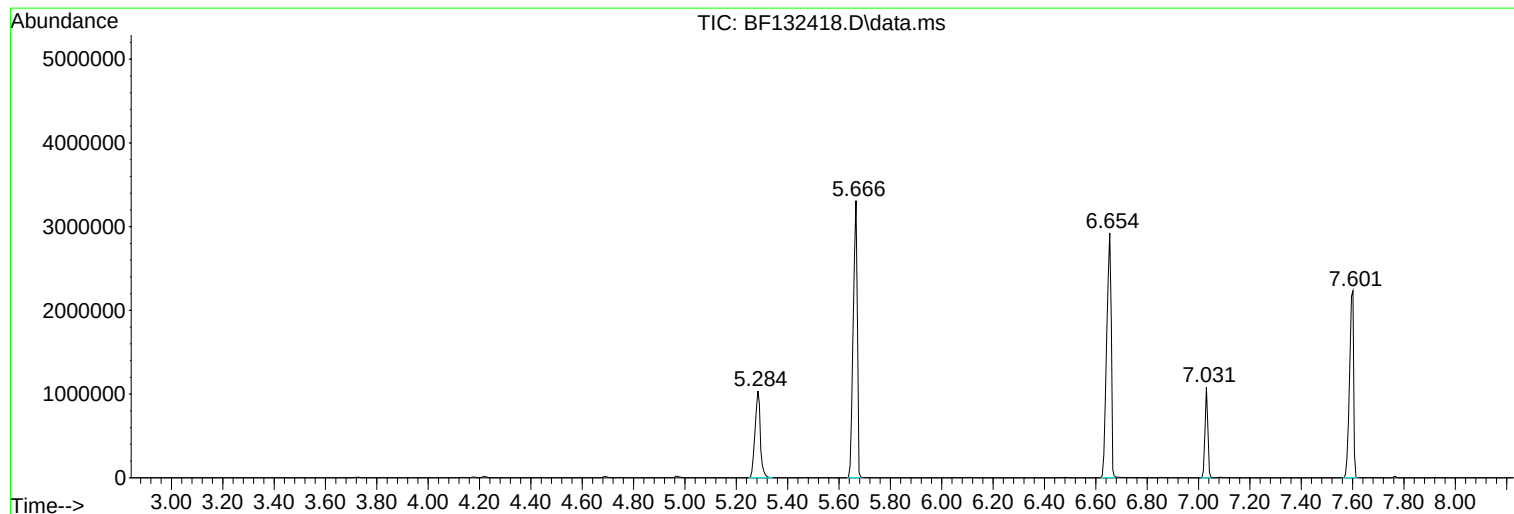
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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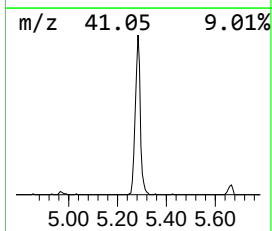
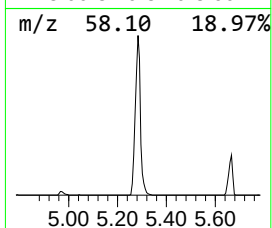
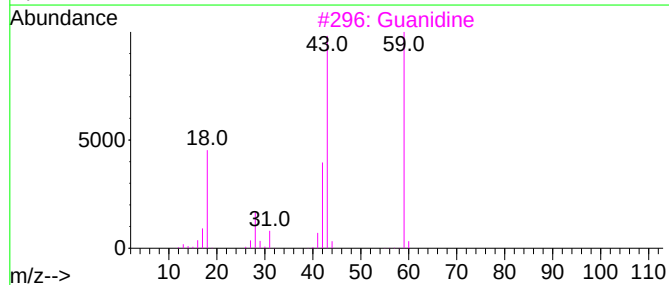
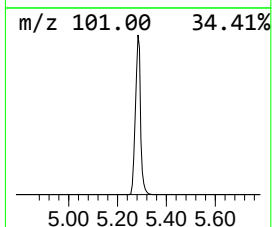
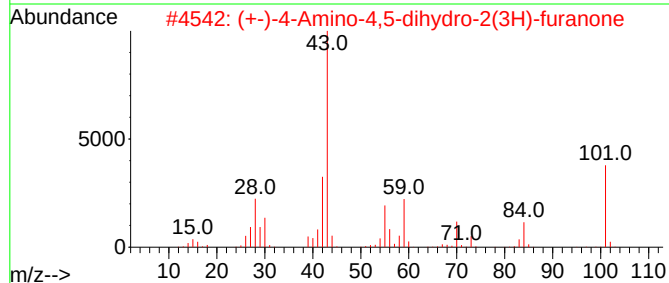
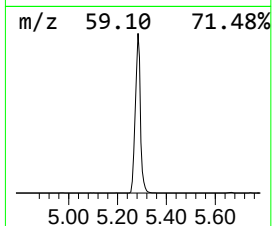
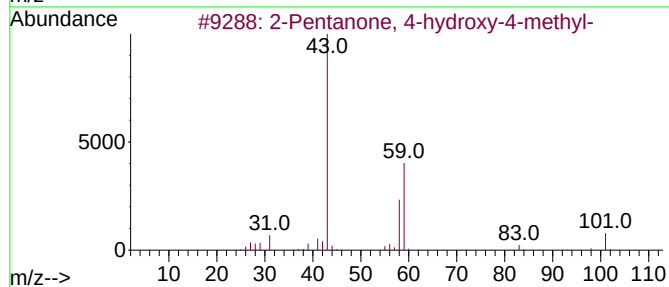
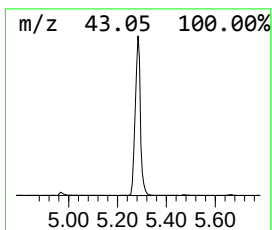
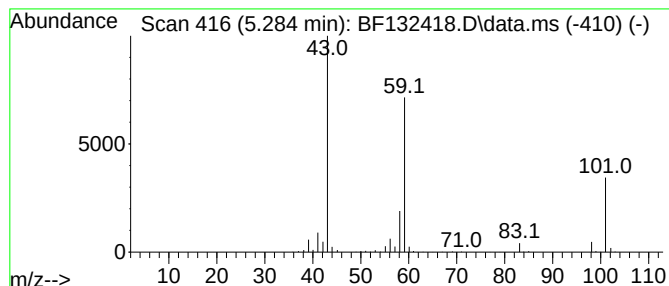
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.284	35.80 ng	1486910	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	59
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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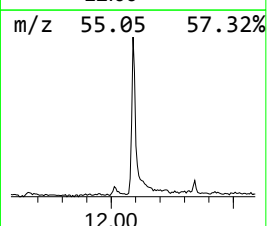
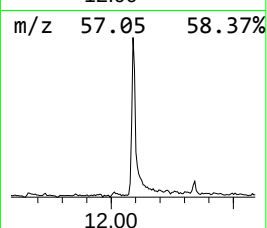
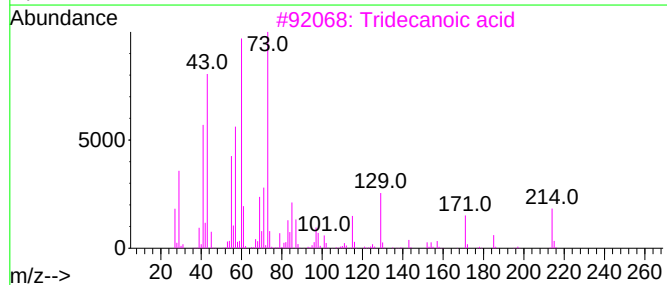
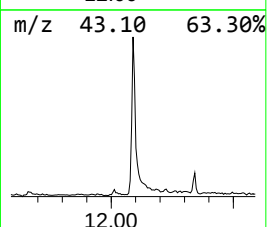
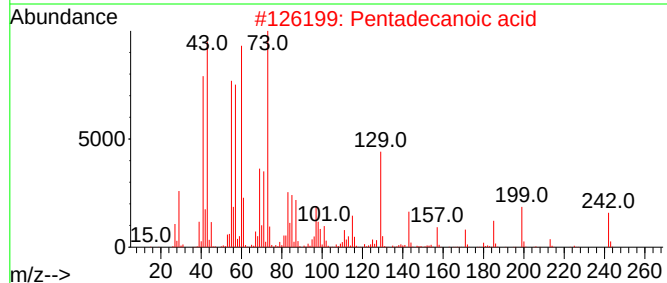
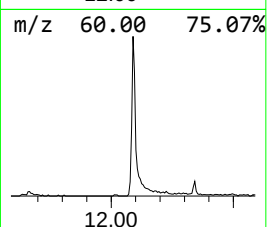
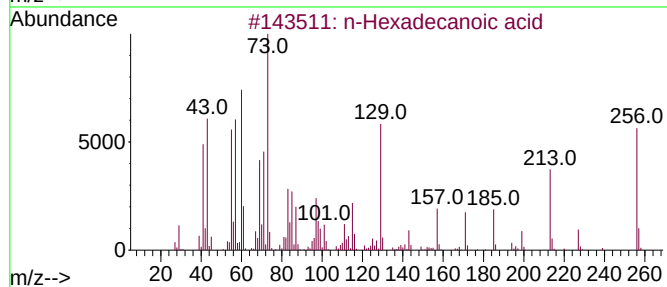
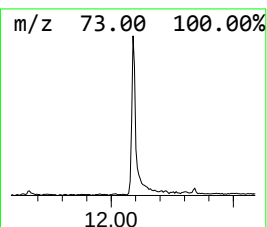
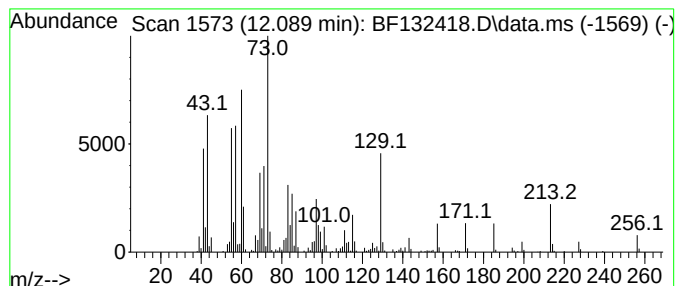
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.089	7.39 ng	506207	Phenanthrene-d10	11.578

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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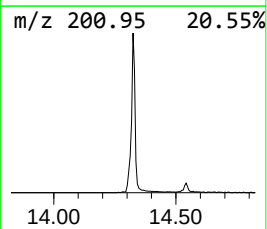
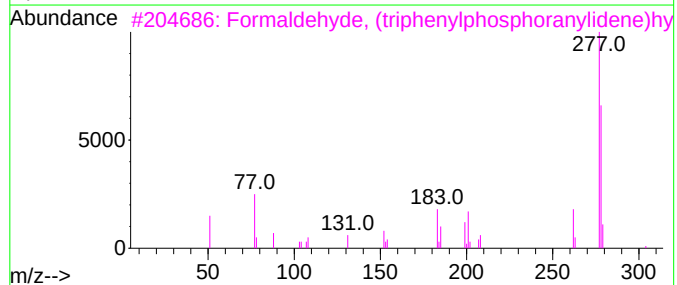
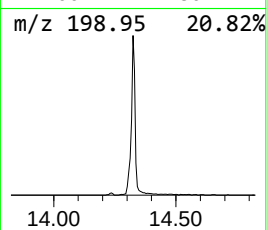
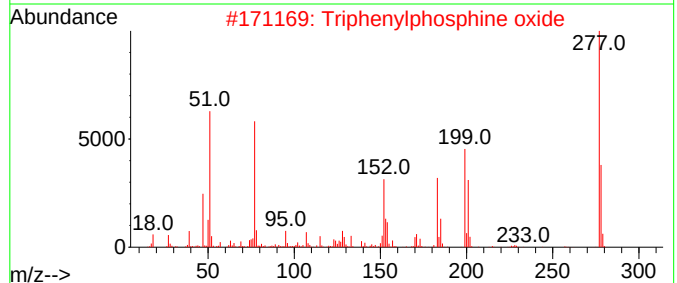
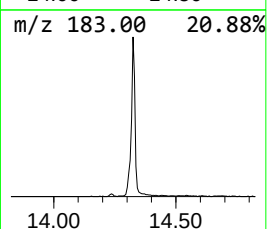
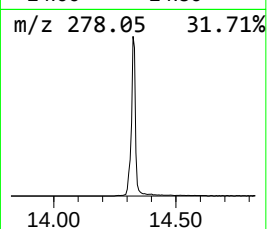
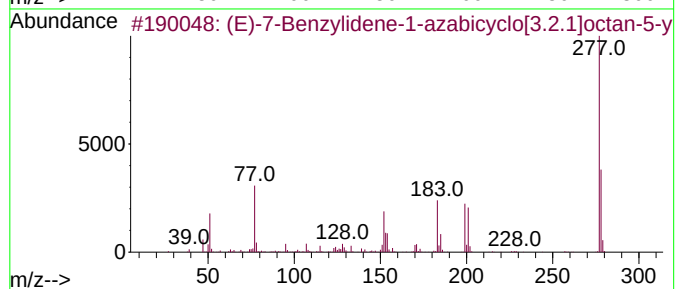
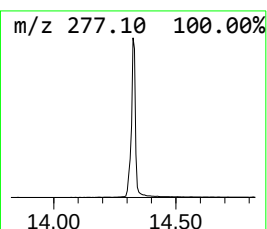
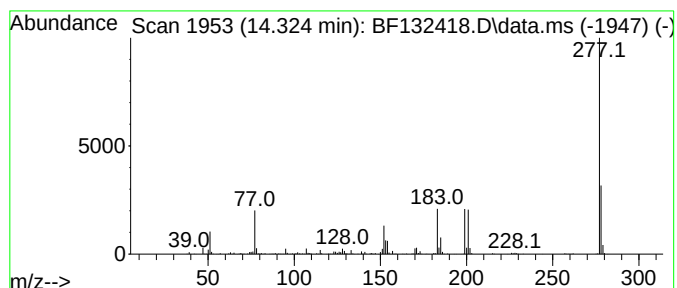
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (E)-7-Benzylidene-1-azabicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.325	17.67 ng	1084970	Chrysene-d12	14.236
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293 C15H19NO3S	1000483-83-4	91
2	Triphenylphosphine oxide	278 C18H15OP	000791-28-6	83
3	Formaldehyde, (triphenylphosphor...	304 C19H17N2P	015990-54-2	42
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277 C16H15BCo	036682-12-9	37
5	1H-Indole-3-acetic acid, 5-[(tri...	277 C14H19NO3Si	072101-35-0	23



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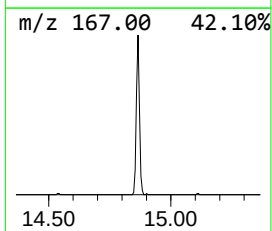
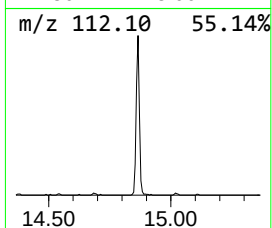
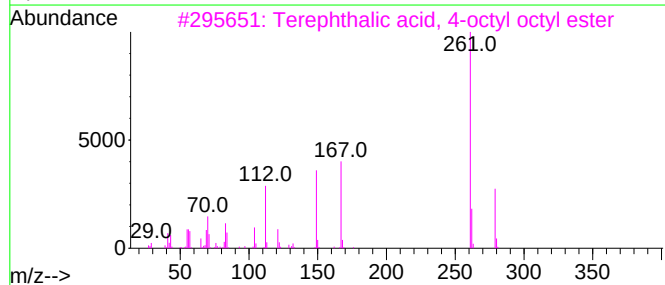
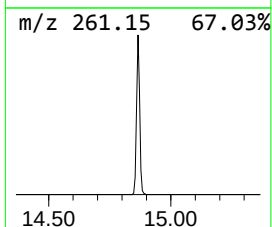
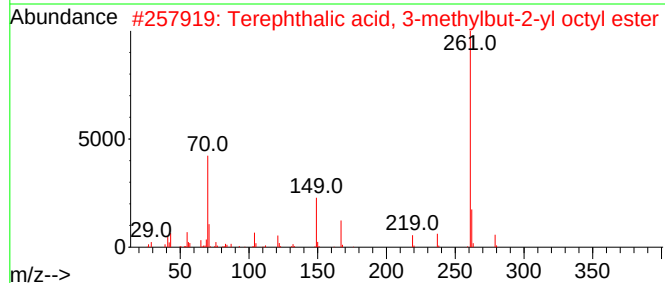
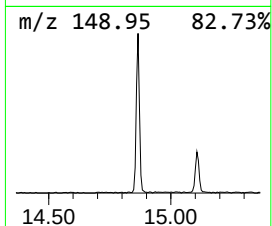
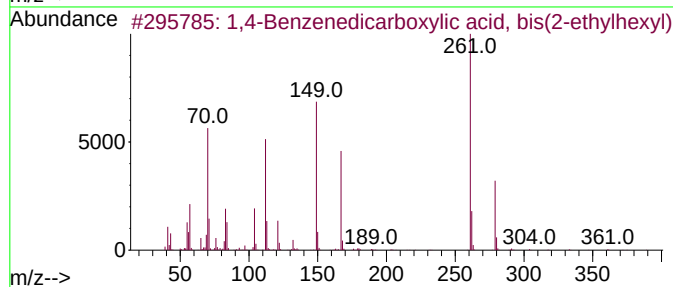
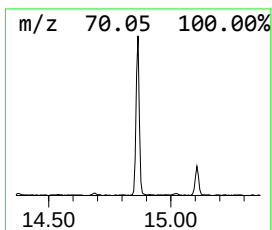
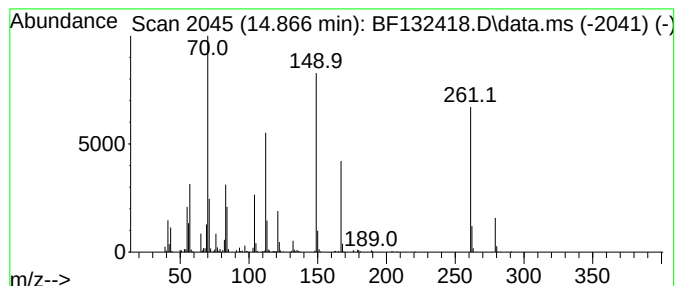
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.866	6.99 ng	429161	Chrysene-d12	14.236	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
3	Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	68
4	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	64
5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	59



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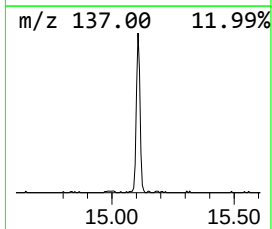
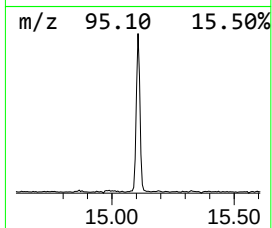
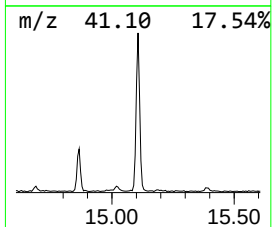
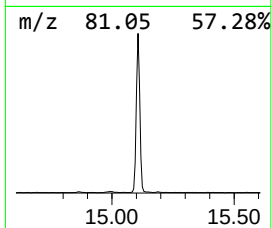
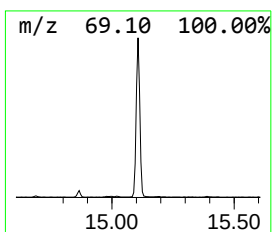
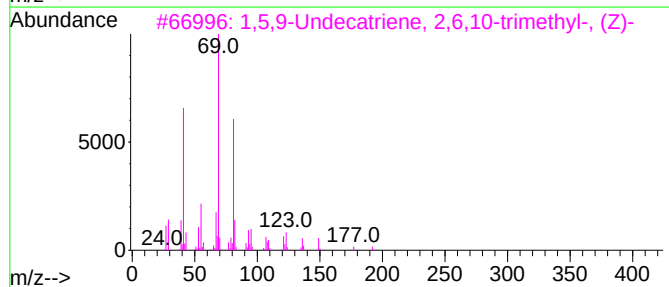
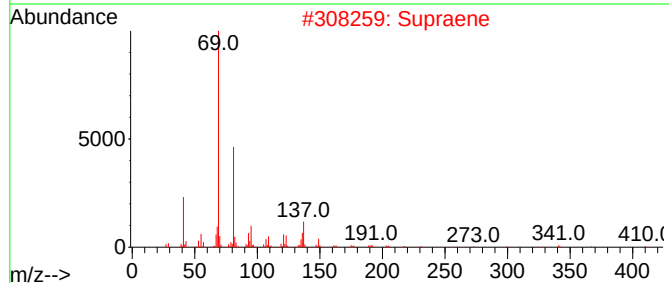
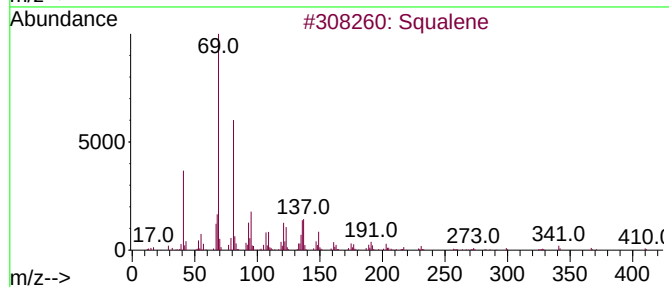
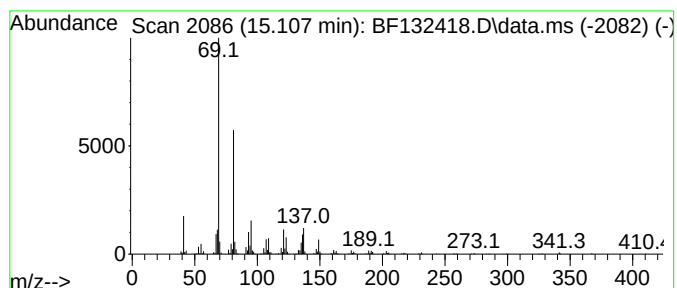
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.107	13.24 ng	822433	Perylene-d12	15.801

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	98
2			Supraene	410	C30H50	007683-64-9	91
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	86
4			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.284	35.8	ng	1486910	1	7.031	830568	20.0
n-Hexadecanoic ...	12.089	7.4	ng	506207	4	11.578	1369720	20.0
(E)-7-Benzylide...	14.325	17.7	ng	1084970	5	14.236	1228000	20.0
1,4-Benzenedica...	14.866	7.0	ng	429161	5	14.236	1228000	20.0
Squalene	15.107	13.2	ng	822433	6	15.801	1242310	20.0