

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021723\
 Data File : BP013849.D
 Acq On : 17 Feb 2023 17:23
 Operator : CG/JU
 Sample : 01581-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 MH-C

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_P\Methods\8270E-BP021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013849.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.175	332	338	349	rBV	1093371	1519569	18.40%	3.400%
2	5.646	411	418	435	rBV	2659704	3899591	47.21%	8.725%
3	7.258	680	692	711	rBV	2434619	3914285	47.39%	8.758%
4	8.111	829	837	844	rBV	565872	930548	11.27%	2.082%
5	9.281	1027	1036	1049	rBV	1437113	2396343	29.01%	5.362%
6	10.934	1309	1317	1329	rBV	690636	1194663	14.46%	2.673%
7	13.369	1722	1731	1744	rBV	3799053	5558695	67.29%	12.438%
8	14.746	1958	1965	1973	rBV	1008277	1476959	17.88%	3.305%
9	16.098	2189	2195	2202	rBV	79810	114127	1.38%	0.255%
10	16.234	2210	2218	2239	rBV	2938198	4264169	51.62%	9.541%
11	17.498	2426	2433	2438	rBV	1314002	1805035	21.85%	4.039%
12	18.351	2573	2578	2584	rBV	299763	410151	4.97%	0.918%
13	19.575	2782	2786	2795	rBV2	137532	210960	2.55%	0.472%
14	19.845	2827	2832	2839	rVB	56277	97219	1.18%	0.218%
15	20.033	2858	2864	2875	rBV	6792057	8260403	100.00%	18.483%
16	20.692	2972	2976	2980	rVB	210583	249437	3.02%	0.558%
17	21.251	3067	3071	3082	rBV	401978	652681	7.90%	1.460%
18	21.575	3121	3126	3131	rBV	1814782	2401764	29.08%	5.374%
19	21.692	3141	3146	3162	rBV	1606638	2707731	32.78%	6.059%
20	24.133	3554	3561	3570	rBV2	1214097	2627607	31.81%	5.879%

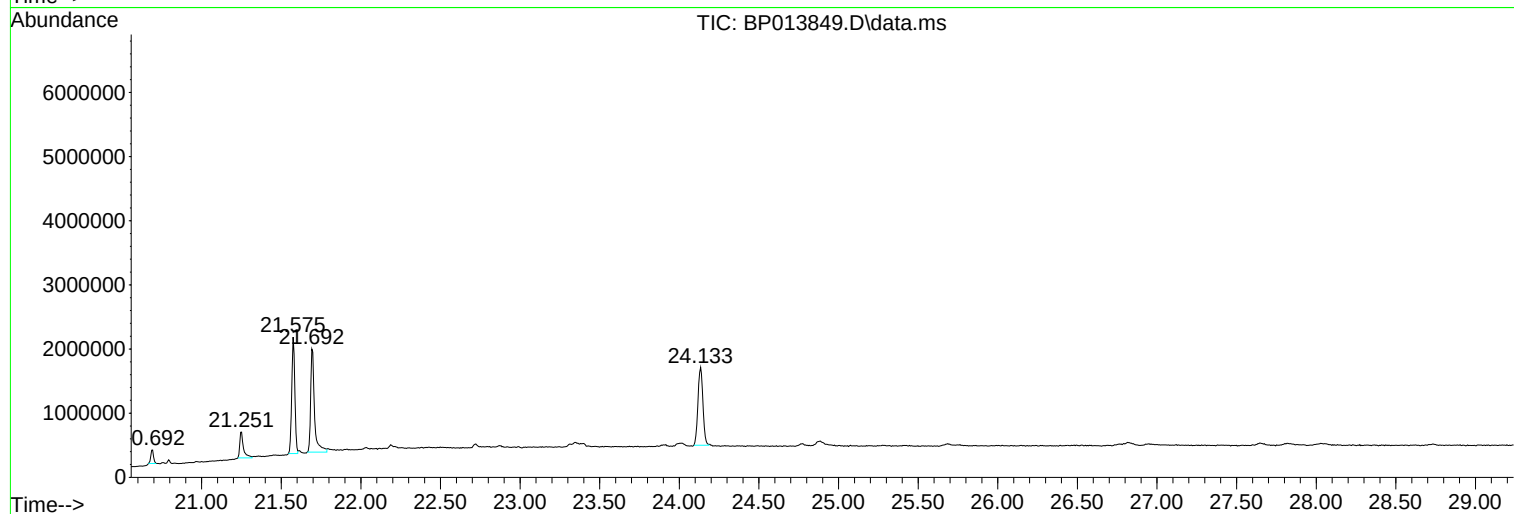
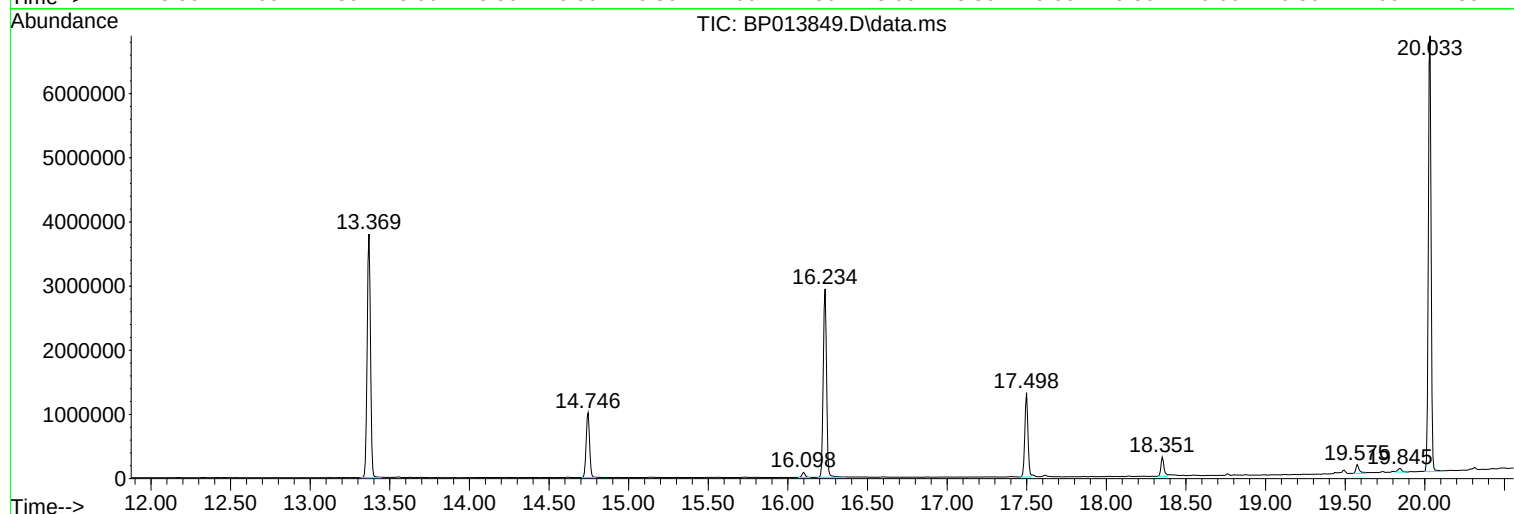
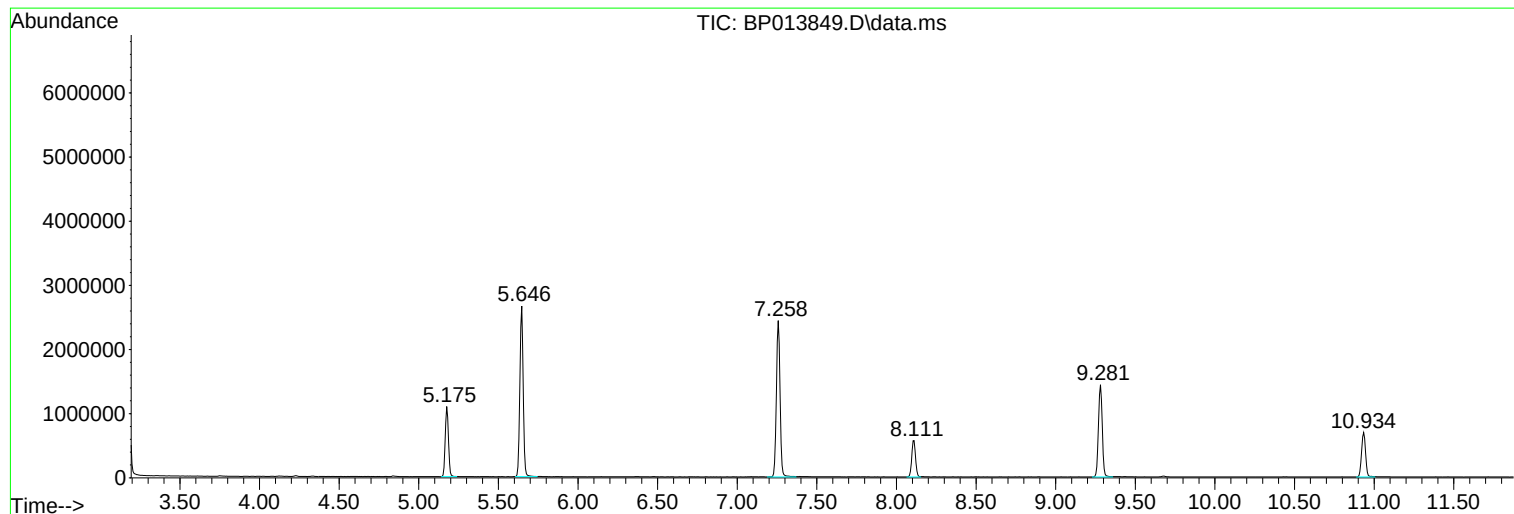
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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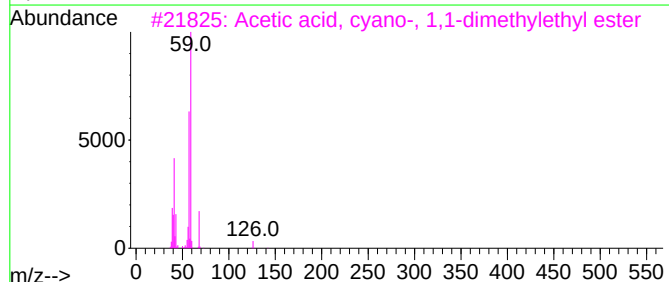
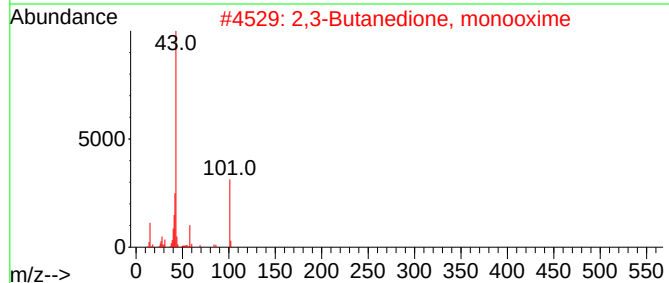
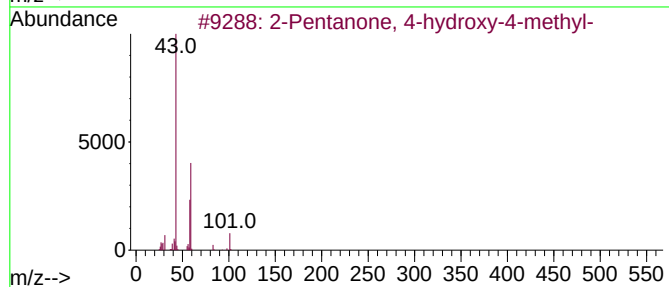
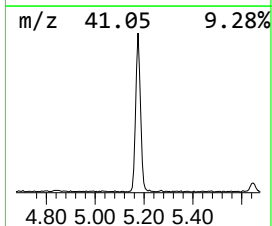
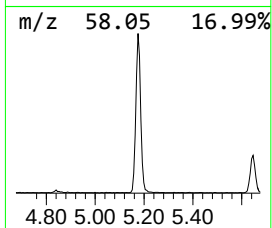
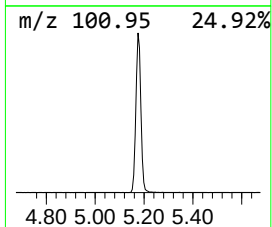
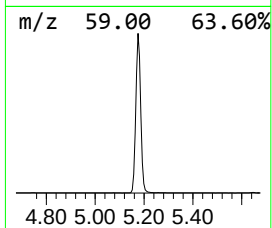
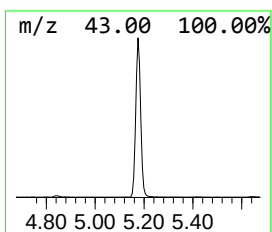
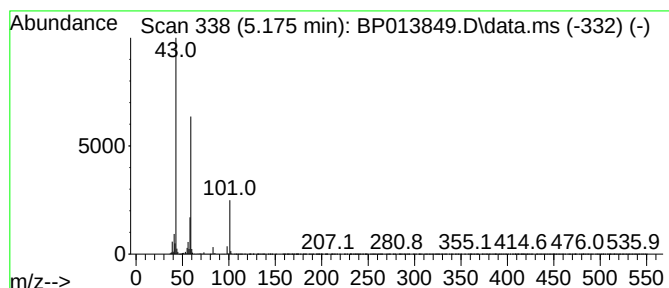
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.175	32.66 ng	1519570	1,4-Dichlorobenzene-d4	8.105

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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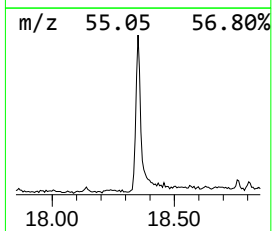
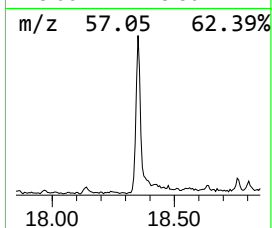
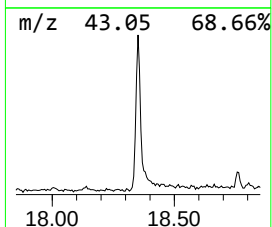
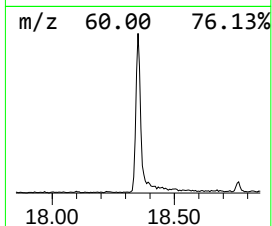
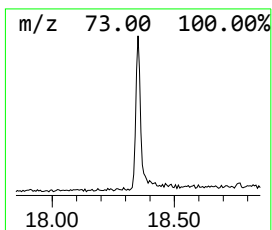
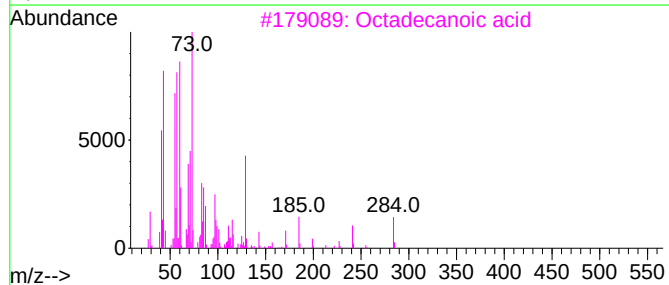
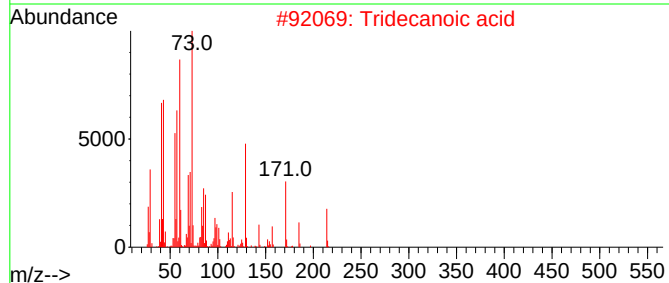
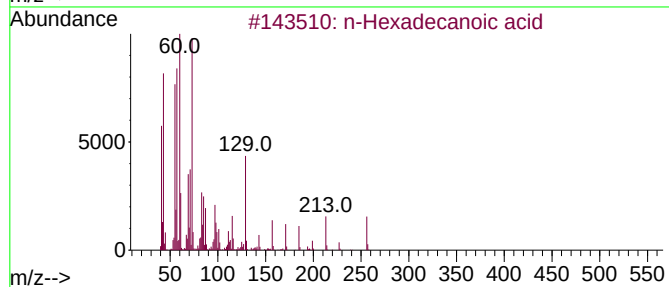
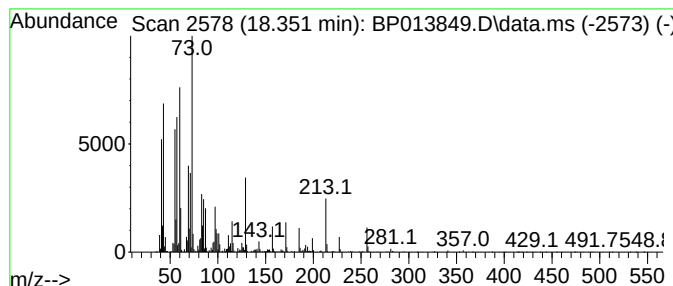
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP021623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.351	4.54 ng	410151	Phenanthrene-d10	17.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Octadecanoic acid	284	C18H36O2	000057-11-4	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	86



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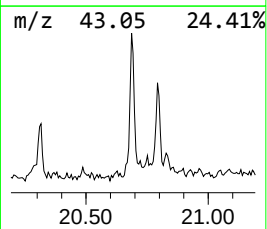
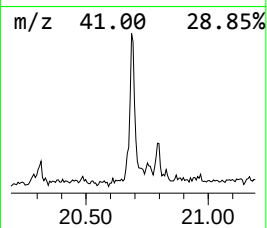
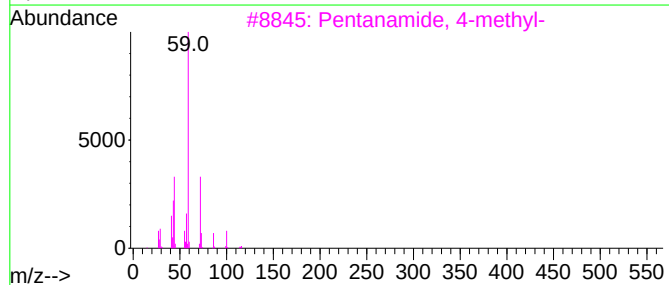
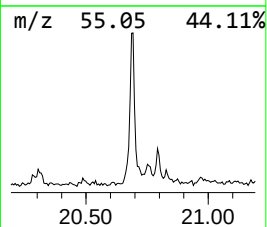
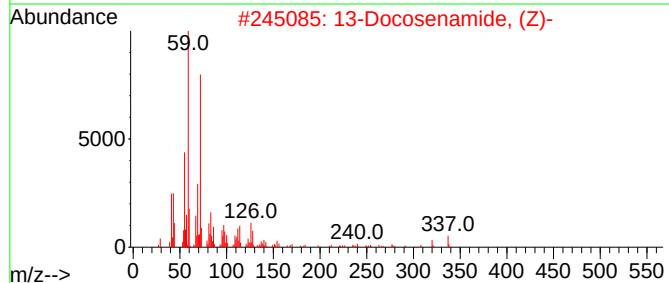
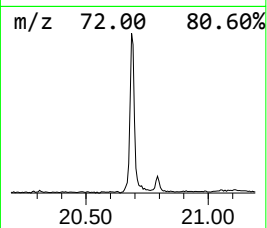
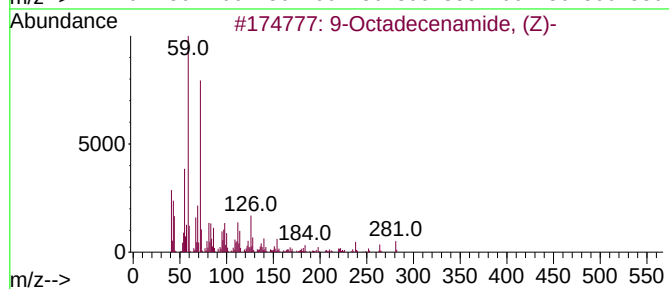
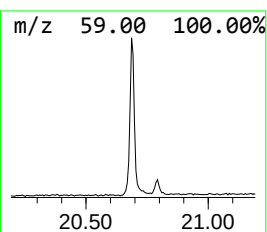
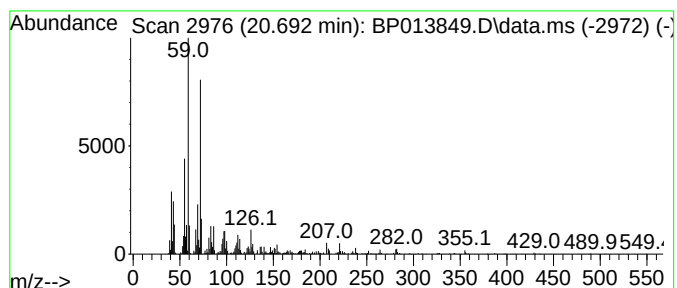
Instrument :
BNA_P
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Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.692	2.08 ng	249437	Chrysene-d12	21.575	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	64
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	47
4	Octadecanamide	283	C18H37NO	000124-26-5	47
5	Octanamide	143	C8H17NO	000629-01-6	43



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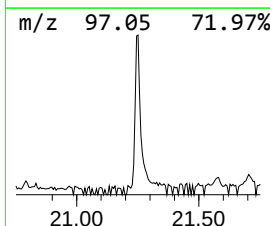
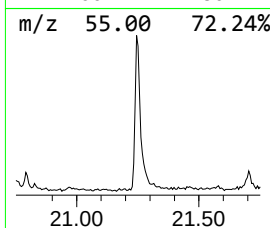
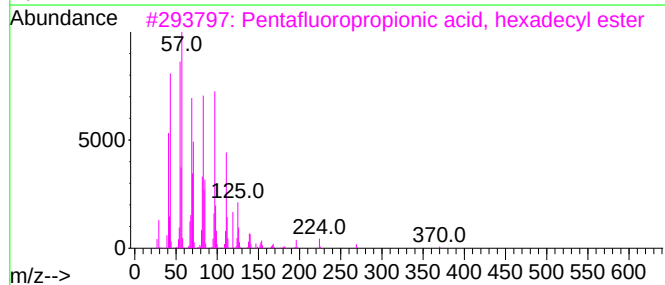
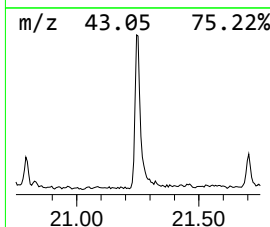
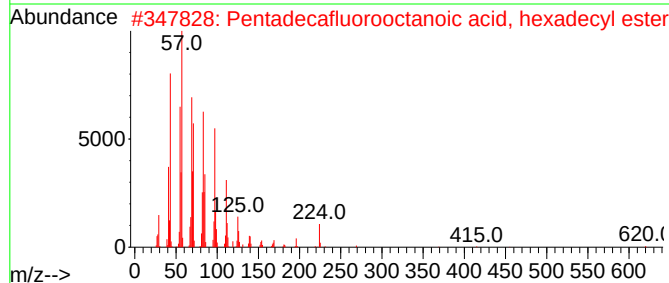
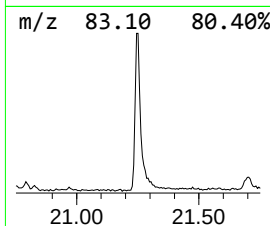
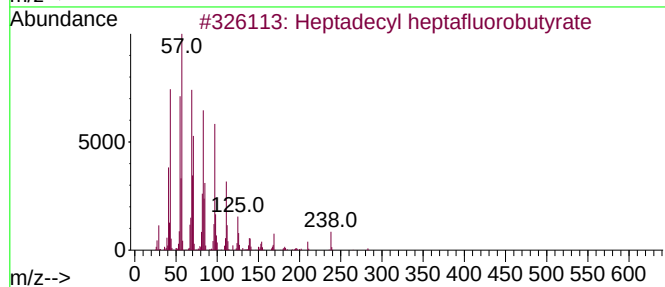
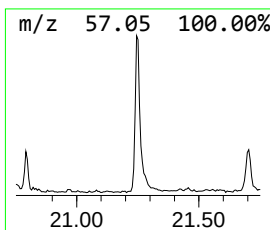
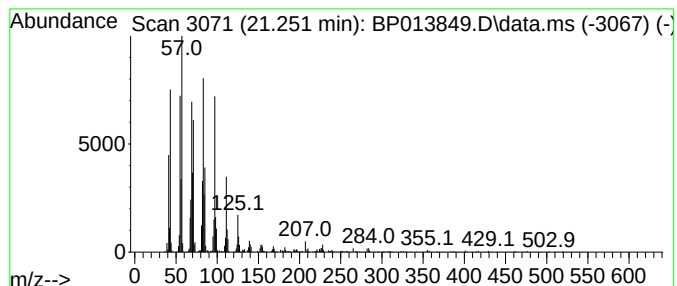
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	5.44 ng	652681	Chrysene-d12	21.575

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	94
3			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91



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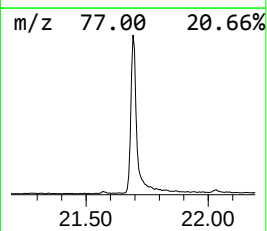
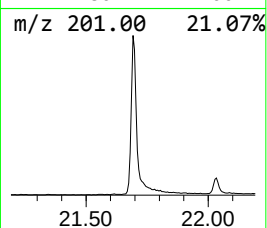
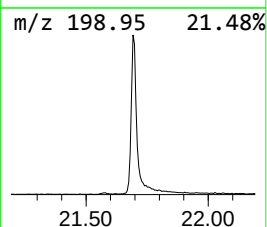
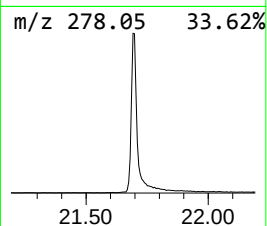
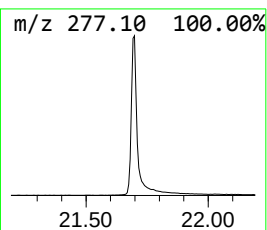
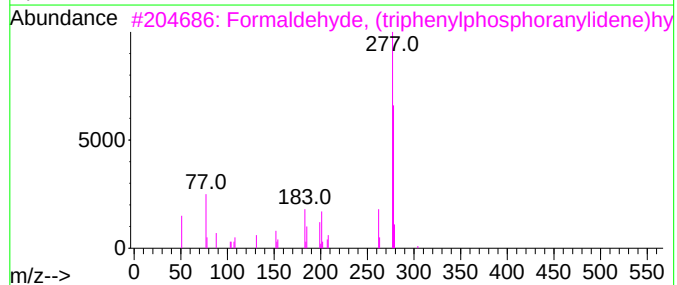
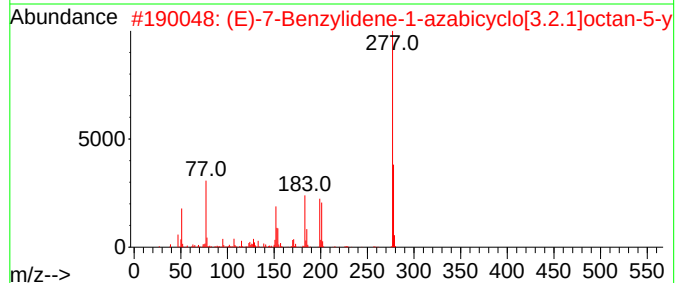
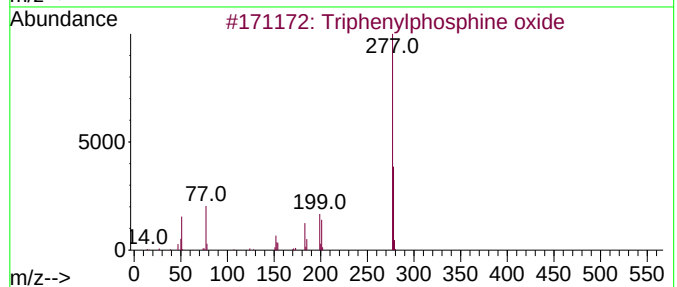
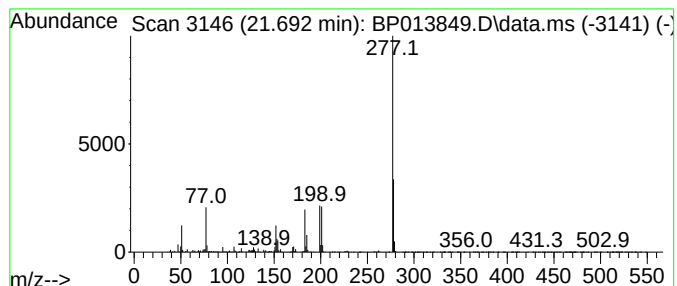
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.692	22.55 ng	2707730	Chrysene-d12	21.575

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	42
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.175	32.7	ng	1519570	1	8.105	930548	20.0
n-Hexadecanoic ...	18.351	4.5	ng	410151	4	17.498	1805040	20.0
9-Octadecenamid...	20.692	2.1	ng	249437	5	21.575	2401760	20.0
Heptadecyl hept...	21.251	5.4	ng	652681	5	21.575	2401760	20.0
Triphenylphosph...	21.692	22.6	ng	2707730	5	21.575	2401760	20.0