

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102922\
 Data File : BM037270.D
 Acq On : 29 Oct 2022 14:40
 Operator : CG/JU
 Sample : N5237-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 LSP-RB

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_M\Methods\8270-BM102822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	314	322	330	rBV	2518033	3410253	13.19%	2.786%
2	5.446	392	401	417	rVB	7170065	9983911	38.60%	8.157%
3	7.046	666	673	685	rBV	4507443	6839429	26.45%	5.588%
4	7.875	806	814	820	rBV	1871006	2926522	11.32%	2.391%
5	8.975	993	1001	1006	rBV	242882	398823	1.54%	0.326%
6	9.045	1006	1013	1032	rVB	6701356	10606289	41.01%	8.665%
7	10.675	1283	1290	1296	rBV	2390029	3867926	14.96%	3.160%
8	12.863	1658	1662	1672	rBV	163051	268098	1.04%	0.219%
9	13.133	1699	1708	1723	rBV	15901990	23348420	90.28%	19.076%
10	14.504	1934	1941	1949	rBV	3159960	4593291	17.76%	3.753%
11	15.992	2187	2194	2212	rBV	10007617	14586515	56.40%	11.917%
12	17.245	2401	2407	2419	rBV	3330821	4726359	18.27%	3.861%
13	17.915	2516	2521	2527	rBV	504248	636678	2.46%	0.520%
14	18.139	2555	2559	2569	rBV3	128232	287556	1.11%	0.235%
15	19.298	2749	2756	2770	rBV2	247801	714559	2.76%	0.584%
16	19.415	2772	2776	2790	rVV2	255089	572532	2.21%	0.468%
17	19.868	2847	2853	2866	rBV	22417816	25862517	100.00%	21.130%
18	21.421	3112	3117	3129	rBV	3413877	4334807	16.76%	3.542%
19	23.780	3512	3518	3527	rVB2	2341980	4432907	17.14%	3.622%

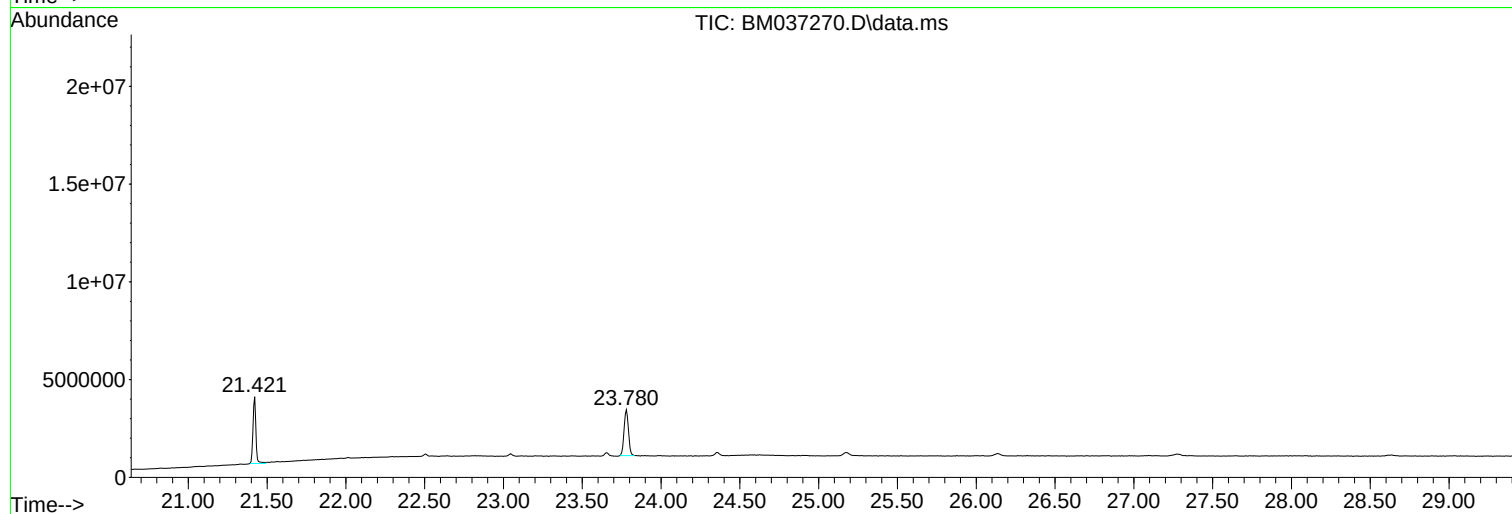
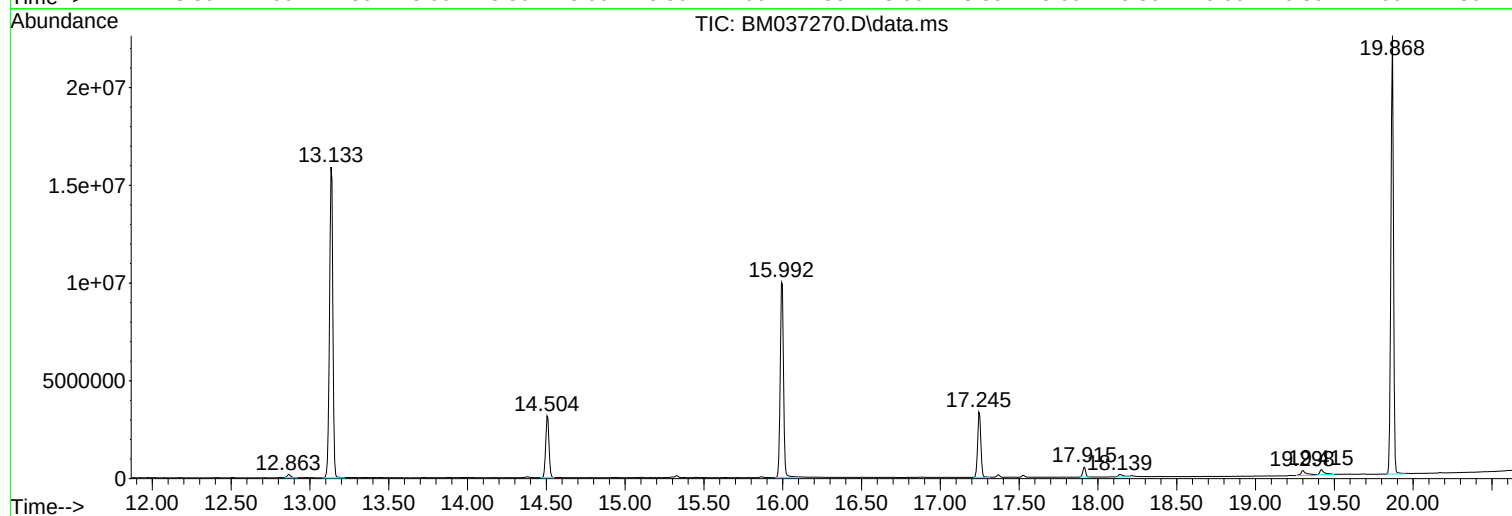
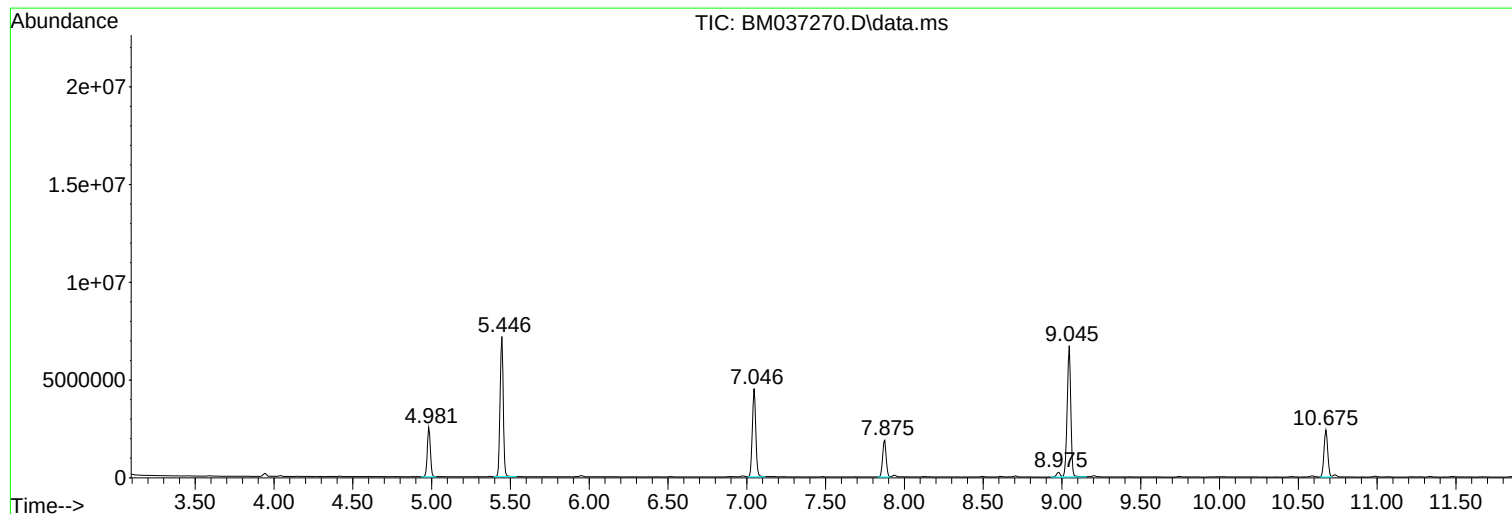
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM037270.D
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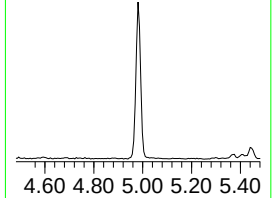
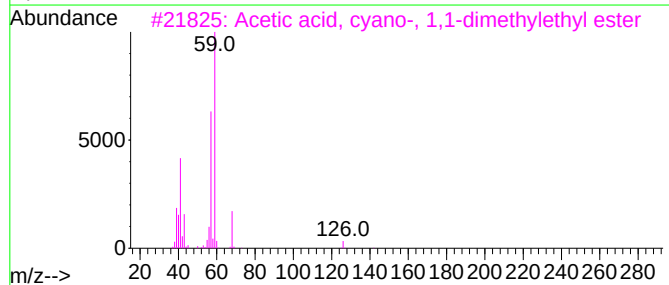
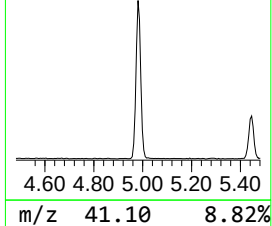
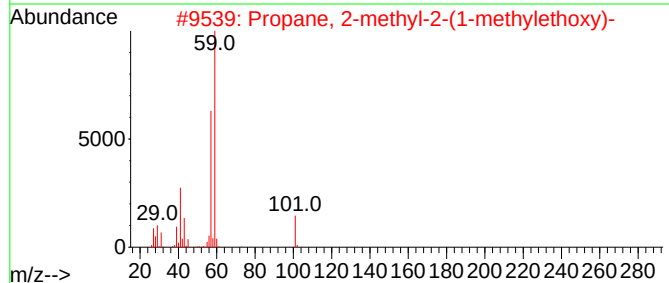
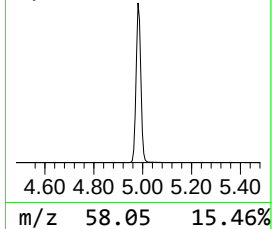
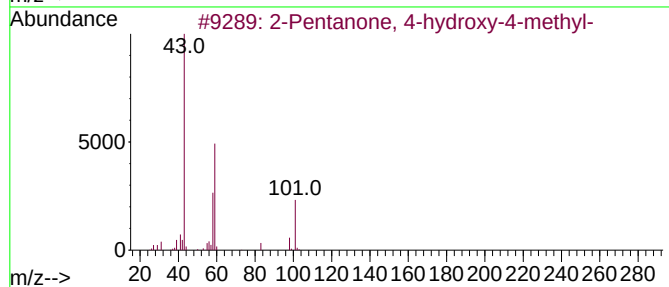
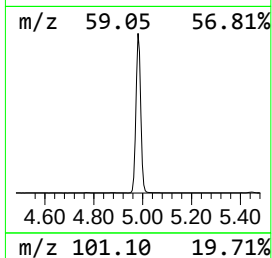
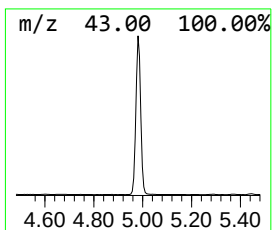
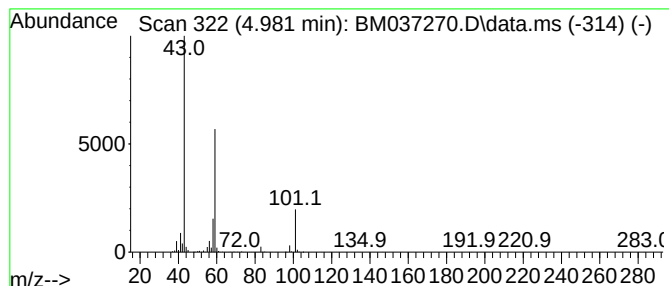
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.981	23.31 ng	3410250	1,4-Dichlorobenzene-d4	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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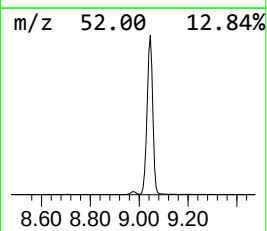
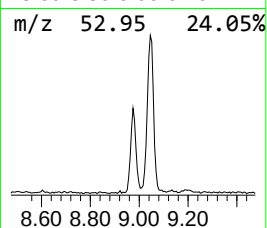
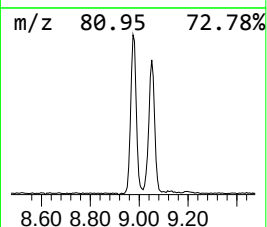
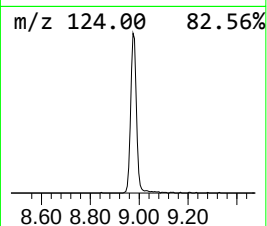
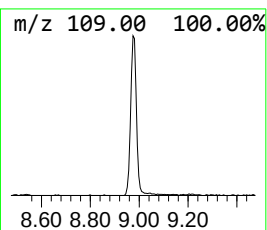
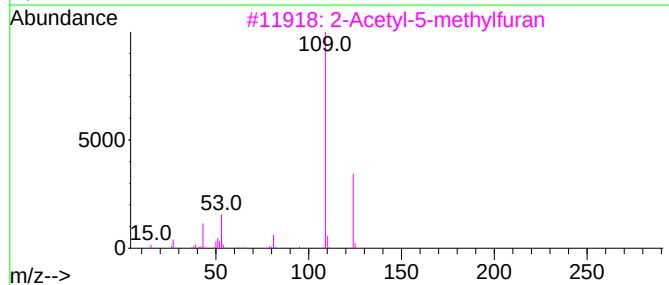
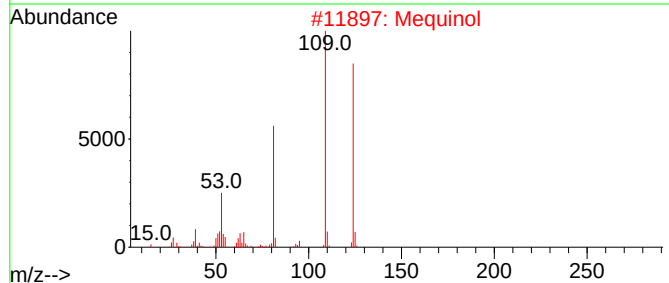
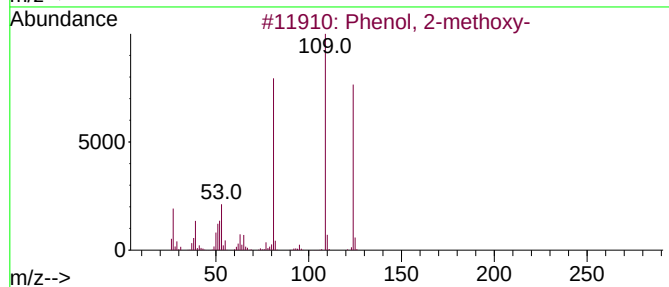
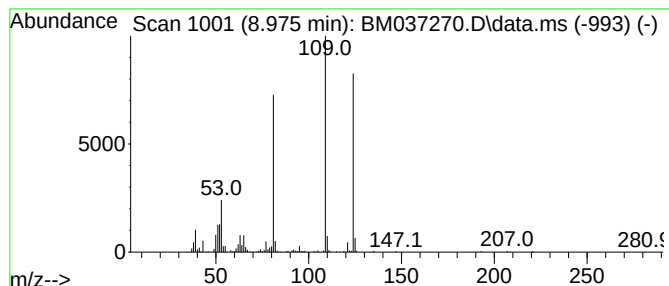
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.975	2.73 ng	398823	1,4-Dichlorobenzene-d4	7.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	97
2			Mequinol	124	C7H8O2	000150-76-5	94
3			2-Acetyl-5-methylfuran	124	C7H8O2	001193-79-9	86
4			5-Ethyl-2-furaldehyde	124	C7H8O2	023074-10-4	86
5			2,3,5-Trimethylcyclopent-2-enone	124	C8H12O	1000427-08-7	80



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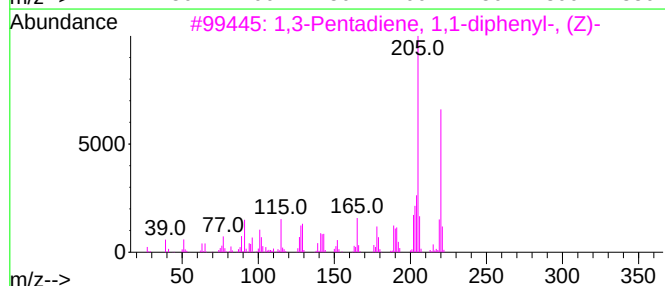
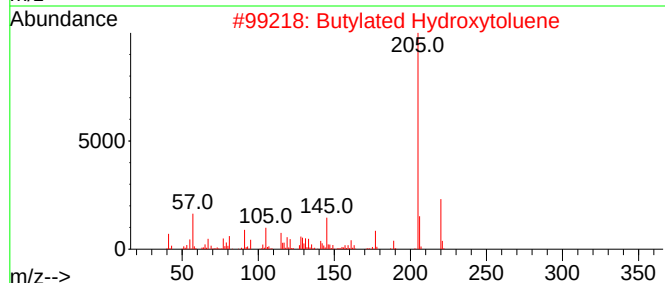
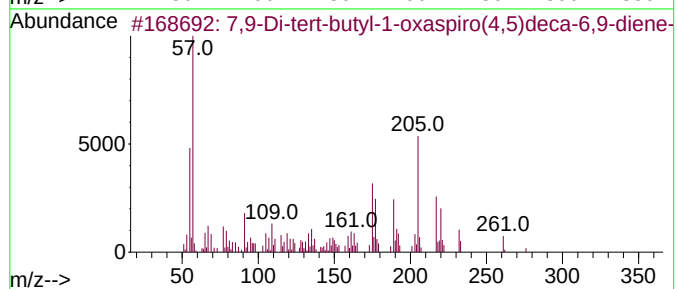
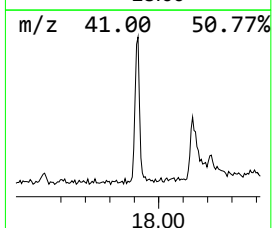
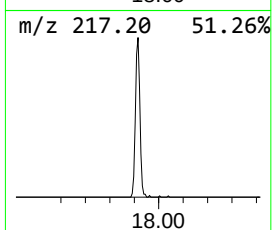
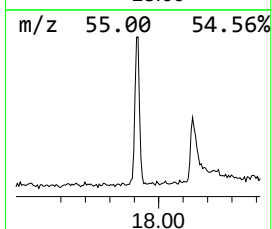
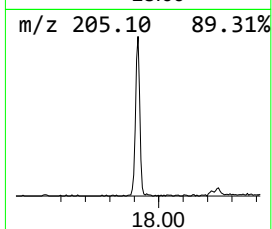
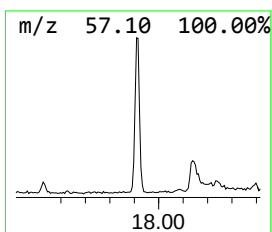
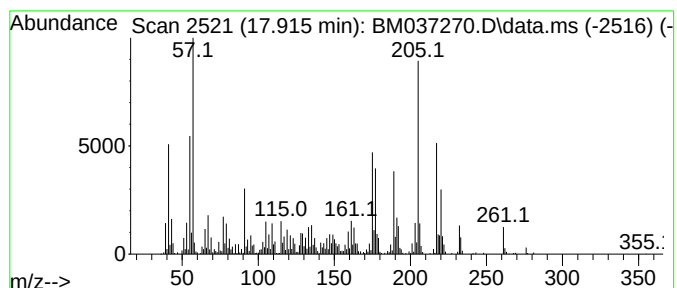
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.915	2.69 ng	636678	Phenanthrene-d10	17.245	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	42
3	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38
4	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	38
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38



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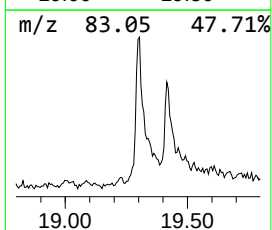
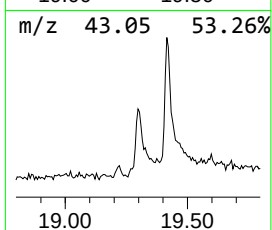
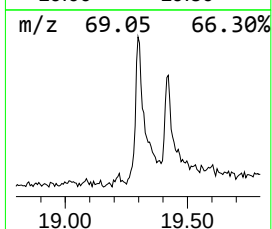
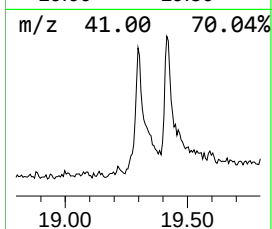
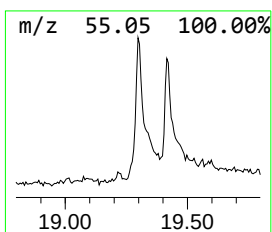
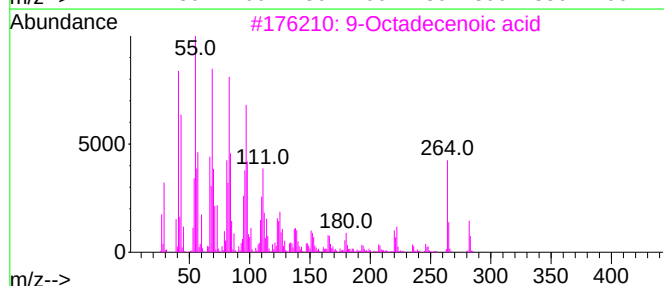
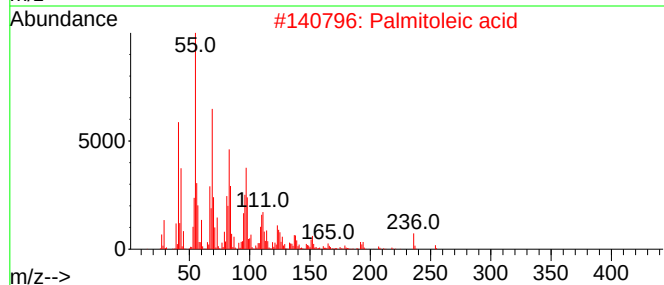
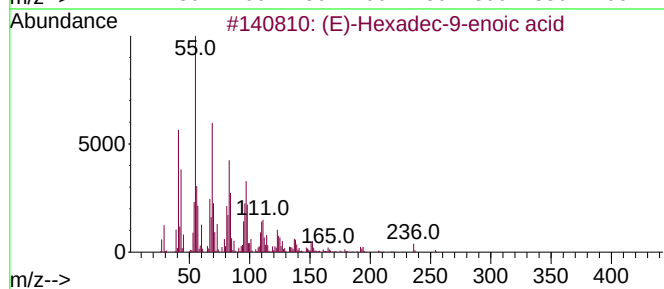
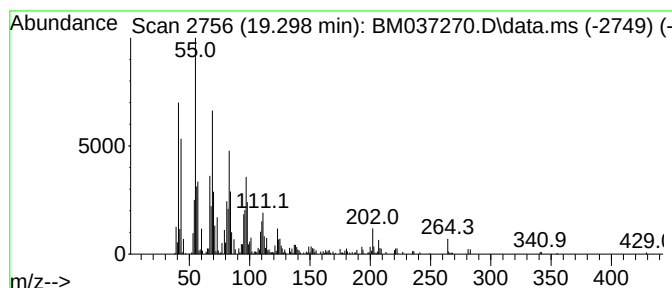
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Peak Number 4 (E)-Hexadec-9-enoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.298	3.02 ng	714559	Phenanthrene-d10	17.245	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	90
2	Palmitoleic acid	254	C16H30O2	000373-49-9	90
3	9-Octadecenoic acid	282	C18H34O2	002027-47-6	87
4	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	87
5	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	87



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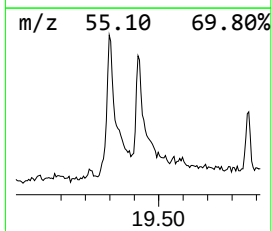
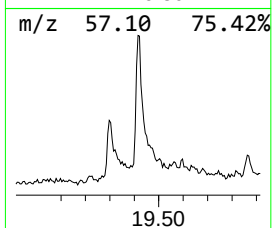
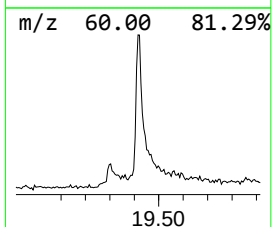
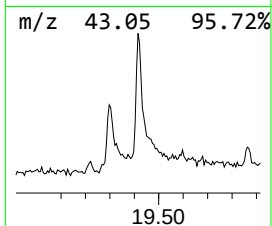
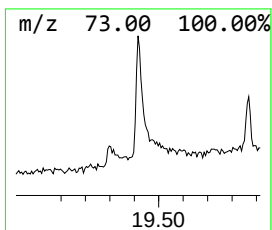
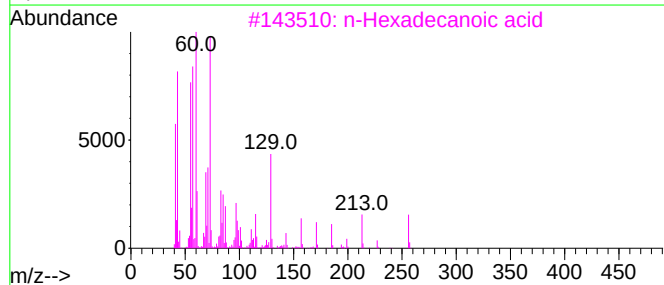
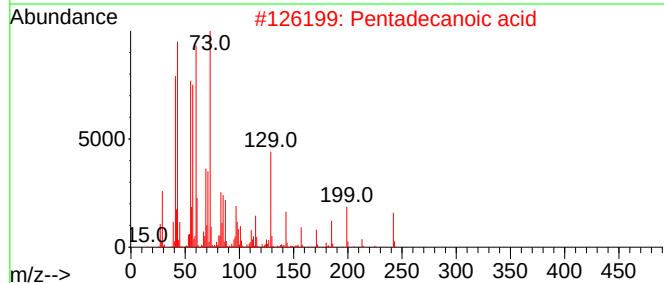
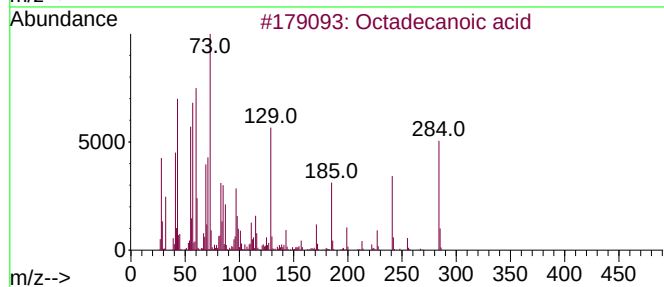
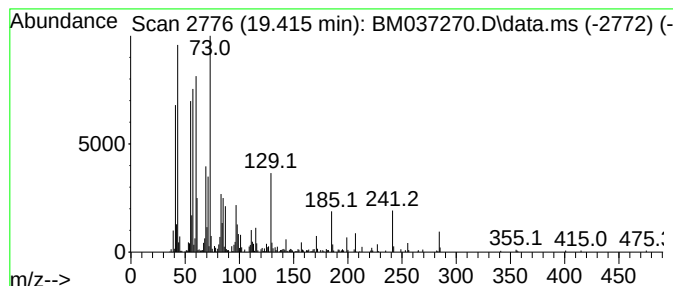
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.415	2.64 ng	572532	Chrysene-d12	21.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.981	23.3	ng	3410250	1	7.875	2926520	20.0
Phenol, 2-methoxy-	8.975	2.7	ng	398823	1	7.875	2926520	20.0
7,9-Di-tert-but...	17.915	2.7	ng	636678	4	17.245	4726360	20.0
(E)-Hexadec-9-e...	19.298	3.0	ng	714559	4	17.245	4726360	20.0
Octadecanoic acid	19.415	2.6	ng	572532	5	21.421	4334810	20.0