

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122021\
 Data File : BM033542.D
 Acq On : 20 Dec 2021 16:20
 Operator : CG/JU
 Sample : M5082-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SASP2-121-1(65-77.7)

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-BM121621.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.025	299	304	315	rBV	133529	191254	12.19%	2.273%
2	5.484	376	382	394	rBV	597542	907047	57.82%	10.778%
3	6.107	481	488	494	rBV	12732	20246	1.29%	0.241%
4	7.090	648	655	670	rBV	573403	954959	60.88%	11.348%
5	7.919	790	796	806	rBV	118070	194041	12.37%	2.306%
6	9.095	989	996	1013	rBV	374311	644066	41.06%	7.653%
7	10.731	1265	1274	1285	rBV	133469	240678	15.34%	2.860%
8	13.189	1686	1692	1707	rBV	839858	1305617	83.23%	15.515%
9	14.566	1919	1926	1937	rVB	196704	302056	19.26%	3.589%
10	16.060	2174	2180	2194	rBV	569115	837648	53.40%	9.954%
11	17.318	2388	2394	2402	rBV	216130	324342	20.68%	3.854%
12	17.695	2453	2458	2467	rVB5	8167	15812	1.01%	0.188%
13	17.983	2502	2507	2515	rVB	63752	79623	5.08%	0.946%
14	18.212	2540	2546	2551	rBV5	8928	15809	1.01%	0.188%
15	19.153	2703	2706	2710	rVB	83577	90832	5.79%	1.079%
16	19.289	2725	2729	2737	rVB2	15513	21486	1.37%	0.255%
17	19.936	2834	2839	2849	rBV	1273012	1568679	100.00%	18.641%
18	21.195	3050	3053	3062	rVB4	50962	81041	5.17%	0.963%
19	21.406	3085	3089	3094	rBV	32854	41225	2.63%	0.490%
20	21.495	3099	3104	3111	rBV	228738	304330	19.40%	3.616%
21	23.900	3507	3513	3524	rBV2	130880	274577	17.50%	3.263%

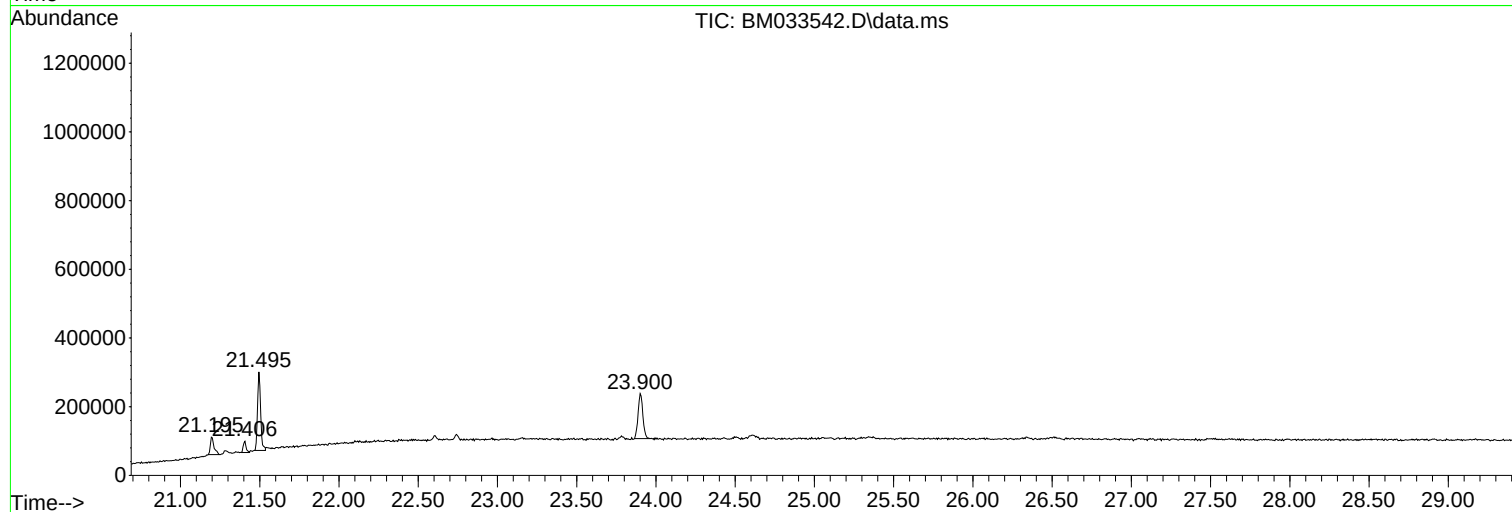
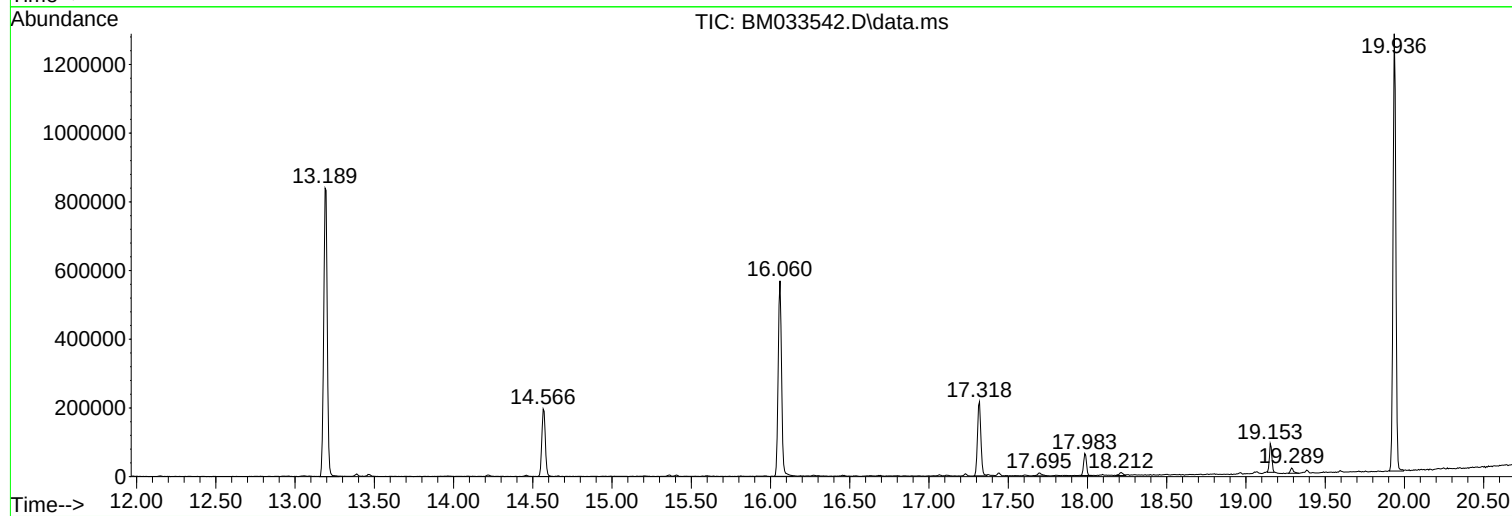
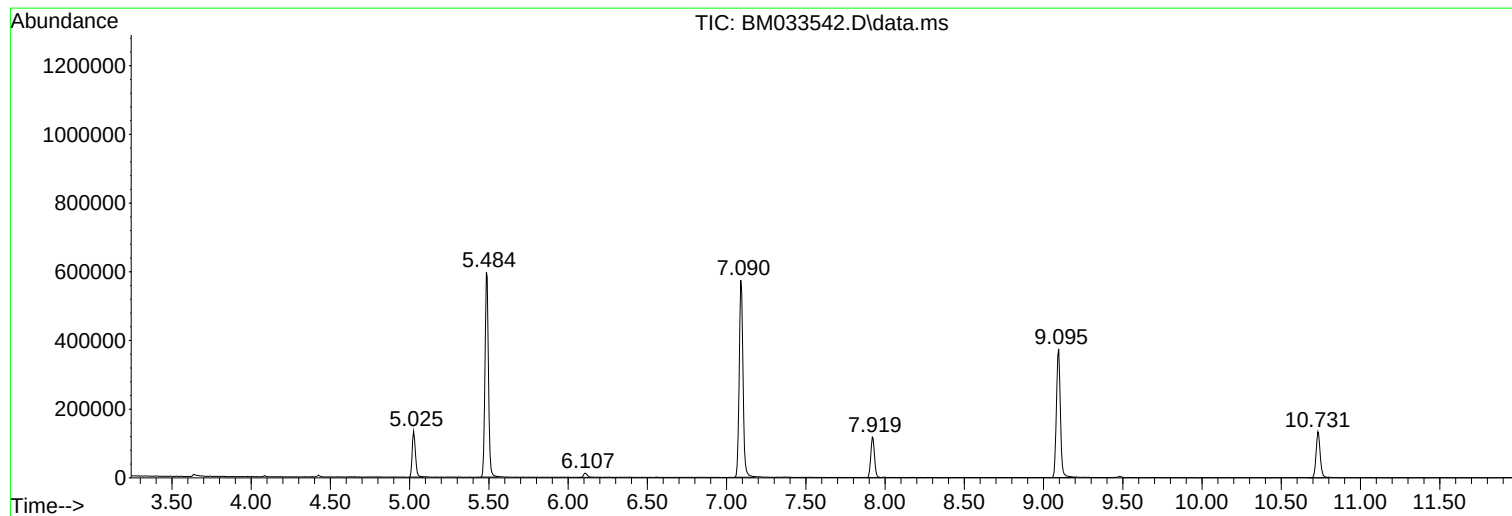
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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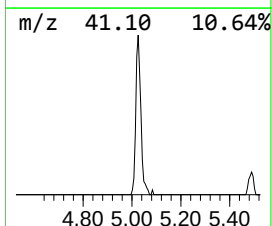
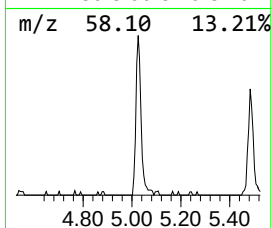
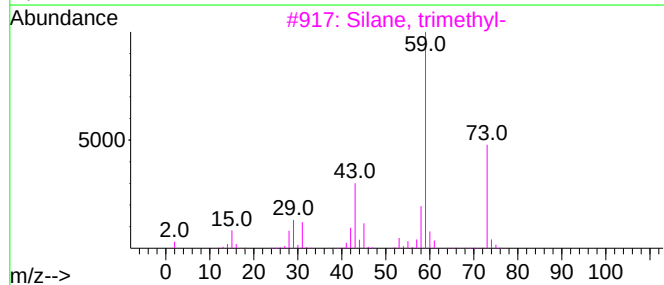
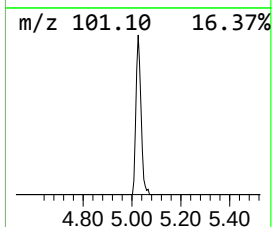
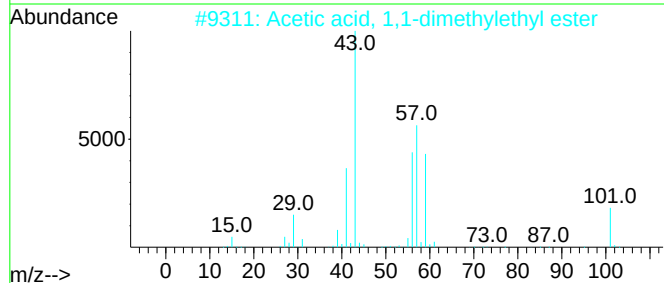
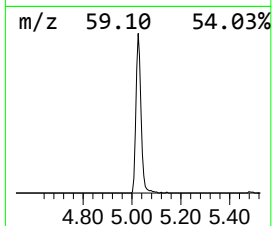
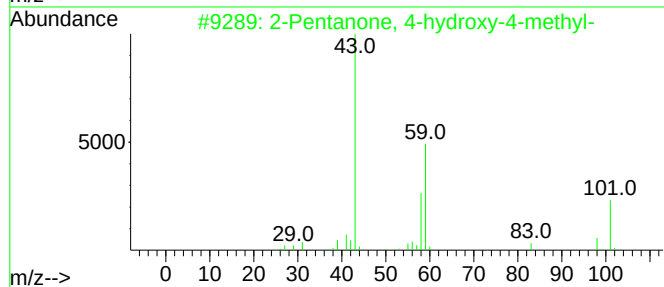
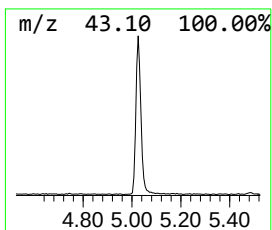
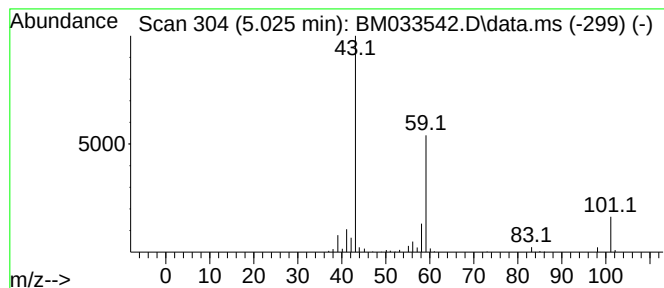
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.025	19.71 ng	191254	1,4-Dichlorobenzene-d4			7.919
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	38
3	Silane, trimethyl-		74	C3H10Si	000993-07-7	25
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
5	Acetamide, N-(cyanomethyl)-		98	C4H6N2O	004814-80-6	9



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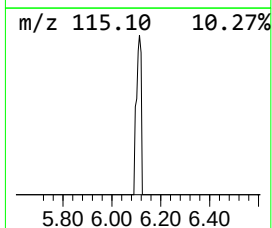
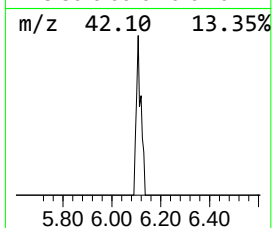
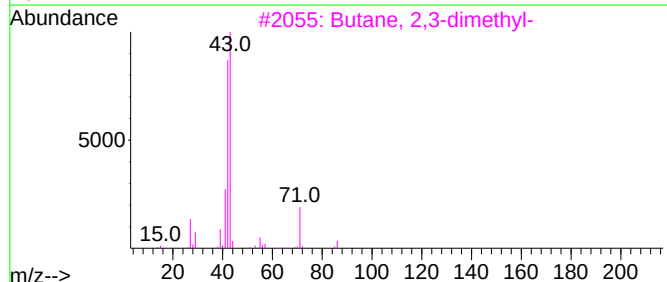
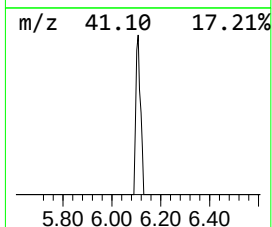
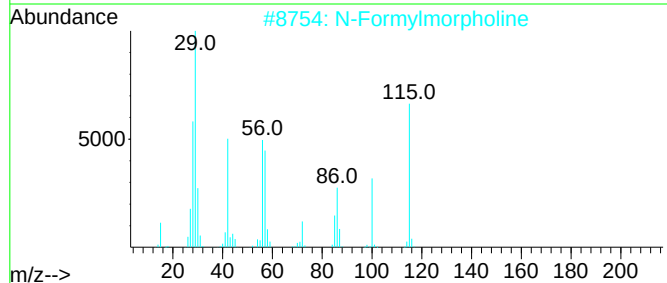
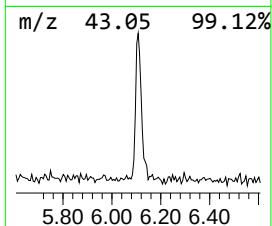
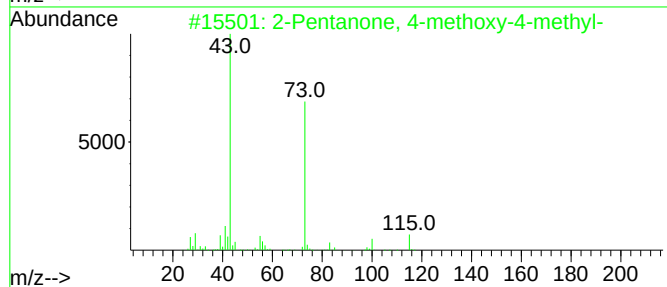
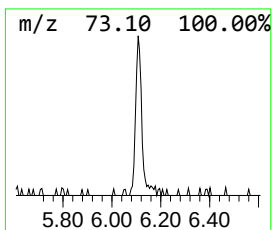
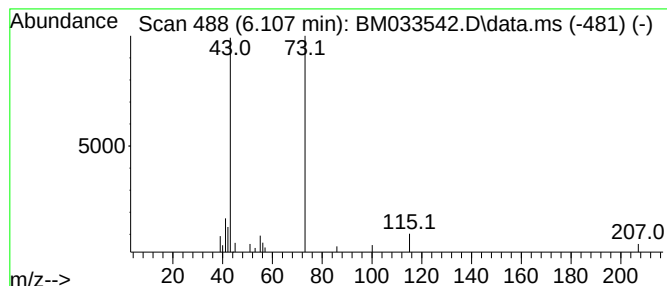
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Peak Number 2 unknown6.107 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.107	2.09 ng	20246	1,4-Dichlorobenzene-d4	7.919

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	42
2			N-Formylmorpholine	115	C5H9NO2	004394-85-8	9
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9
4			1-Amino-3,3-dimethyl-2-butanone	115	C6H13NO	082962-91-2	9
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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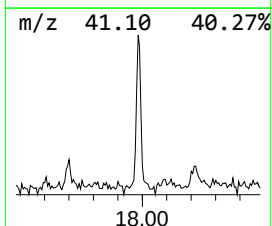
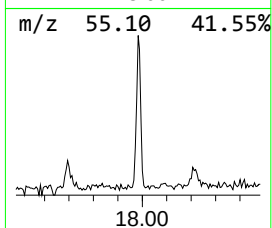
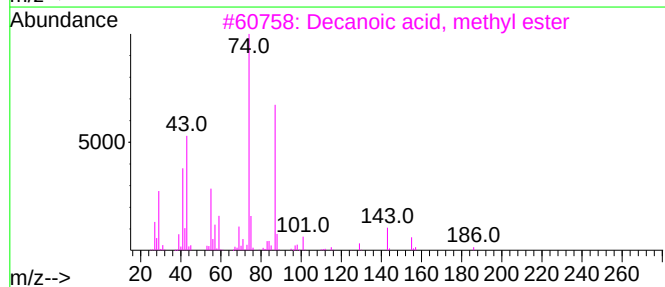
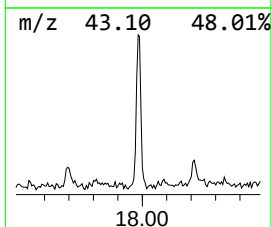
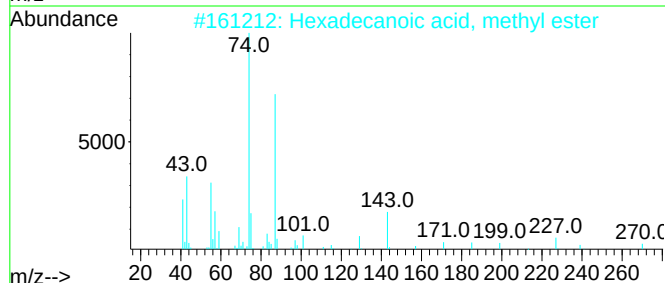
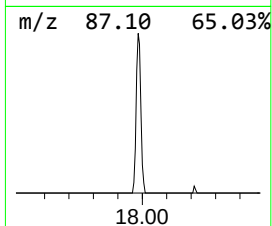
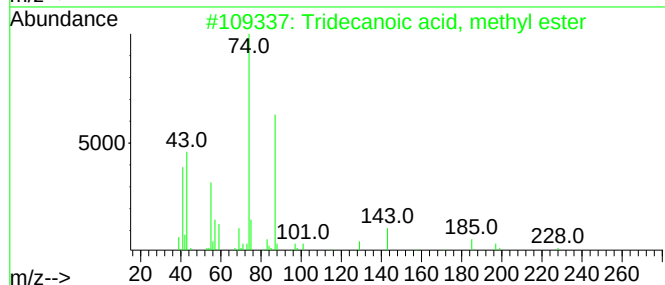
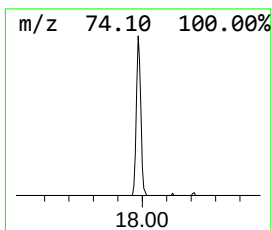
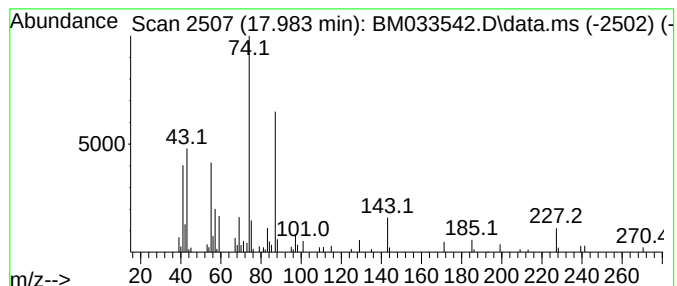
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Peak Number 3 Tridecanoic acid, methyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.983	4.91 ng	79623	Phenanthrene-d10	17.318

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	96
2			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
3			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	93
4			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
5			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	87



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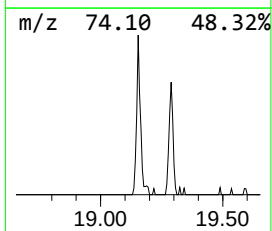
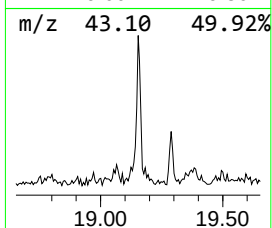
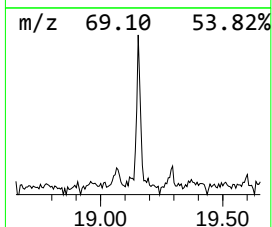
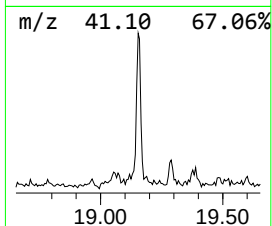
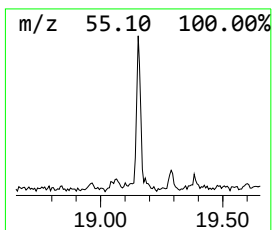
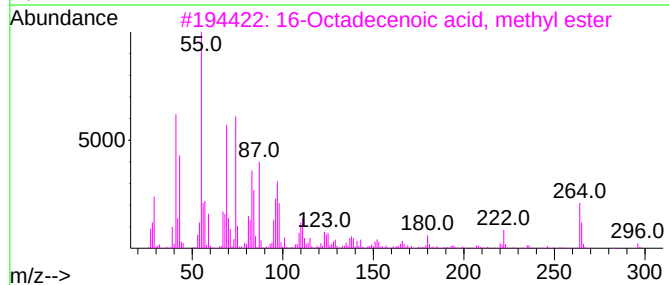
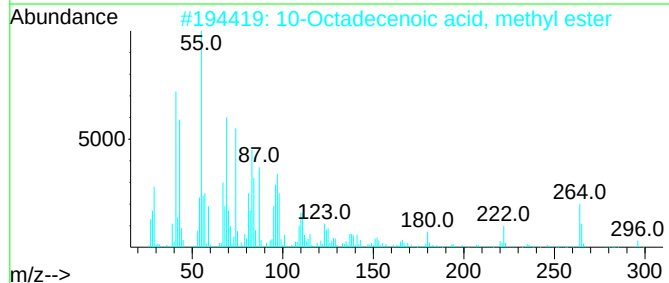
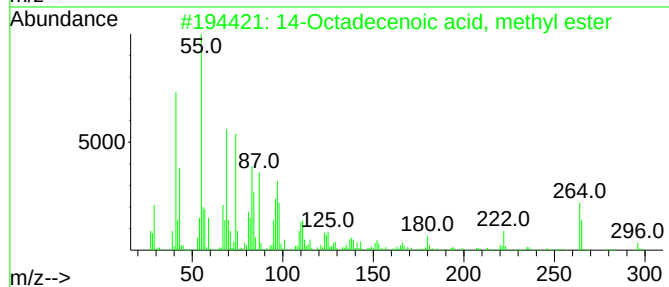
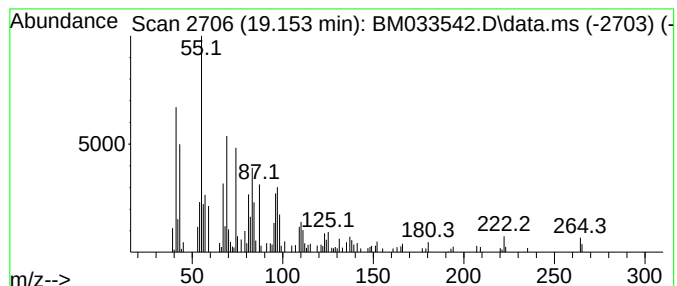
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Peak Number 4 14-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.154	5.60 ng	90832	Phenanthrene-d10	17.318	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	87
4	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	87
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	83



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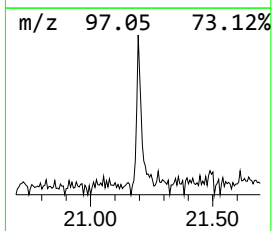
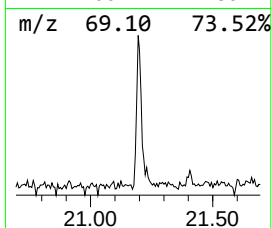
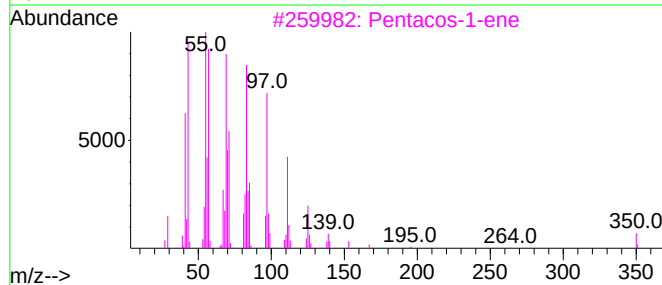
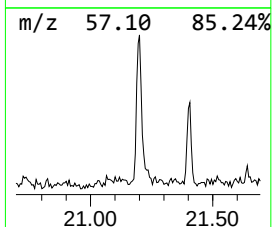
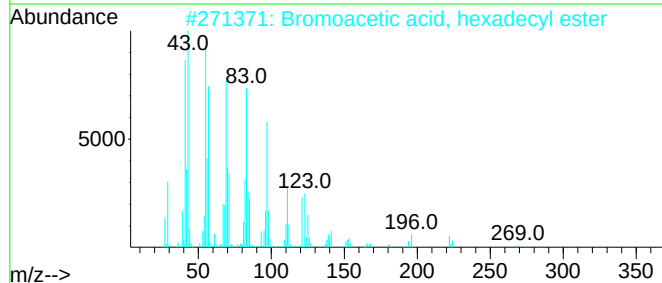
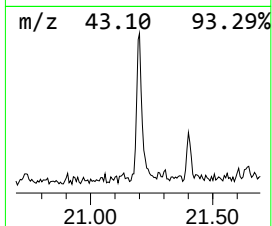
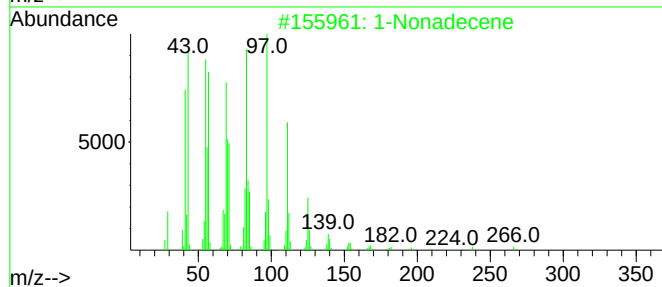
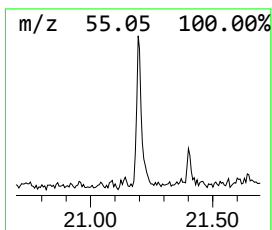
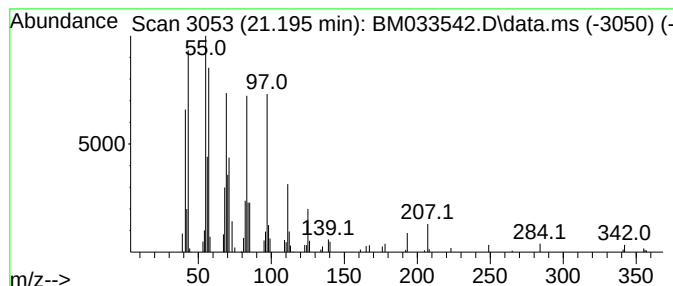
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Peak Number 5 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.195	5.33 ng	81041	Chrysene-d12	21.494

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	91
2	Bromoacetic acid, hexadecyl ester			362	C18H35BrO2	005454-48-8	91
3	Pentacos-1-ene			350	C25H50	016980-85-1	91
4	1-Tetracosene			336	C24H48	010192-32-2	91
5	1-Hexacosene			364	C26H52	018835-33-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.025	19.7	ng	191254	1	7.919	194041	20.0
unknown6.107	6.107	2.1	ng	20246	1	7.919	194041	20.0
Tridecanoic aci...	17.983	4.9	ng	79623	4	17.318	324342	20.0
14-Octadecenoic...	19.154	5.6	ng	90832	4	17.318	324342	20.0
1-Nonadecene	21.195	5.3	ng	81041	5	21.494	304330	20.0