

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057856.D
 Acq On : 24 Jun 2023 00:50
 Operator : CG/JU
 Sample : 03336-16
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-1

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_G\Methods\8270-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057856.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.030	324	330	339	rVB	46711	71158	4.09%	0.646%
2	5.494	403	409	420	rVB	620516	976008	56.11%	8.867%
3	7.087	672	680	690	rVB	620292	1040250	59.81%	9.450%
4	7.921	816	822	829	rVB	170848	280354	16.12%	2.547%
5	9.084	1011	1020	1035	rVB	355707	624140	35.88%	5.670%
6	10.723	1291	1299	1307	rBV	232026	411767	23.67%	3.741%
7	13.179	1710	1717	1726	rBV	897254	1328976	76.41%	12.073%
8	14.554	1945	1951	1960	rVB	367440	550917	31.67%	5.005%
9	15.911	2176	2182	2188	rBV	158702	221283	12.72%	2.010%
10	16.041	2197	2204	2216	rBV	736971	1107970	63.70%	10.065%
11	17.298	2412	2418	2428	rVB	453896	663748	38.16%	6.030%
12	18.185	2564	2569	2580	rBV	155064	233868	13.45%	2.125%
13	19.460	2782	2786	2793	rBV2	43776	64610	3.71%	0.587%
14	19.913	2857	2863	2870	rBV	1331353	1739319	100.00%	15.801%
15	21.205	3079	3083	3091	rVB	83695	125921	7.24%	1.144%
16	21.552	3136	3142	3148	rVB2	428514	671611	38.61%	6.101%
17	22.997	3383	3388	3396	rBV2	47463	102299	5.88%	0.929%
18	24.701	3670	3678	3691	rVB	273606	793486	45.62%	7.208%

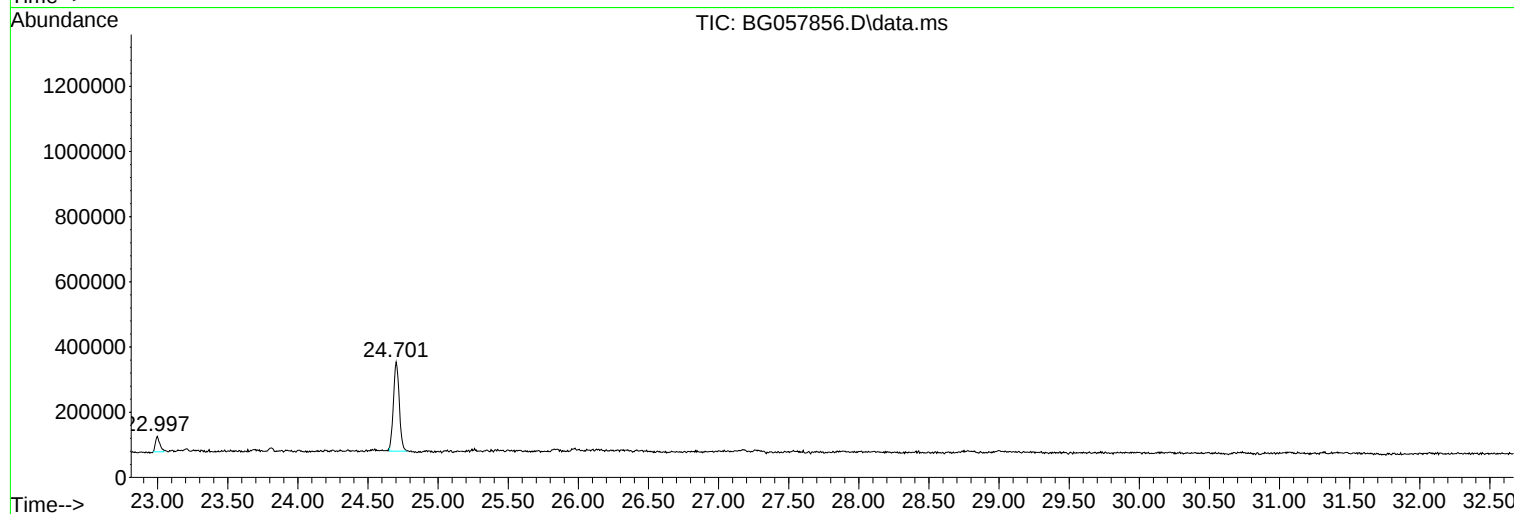
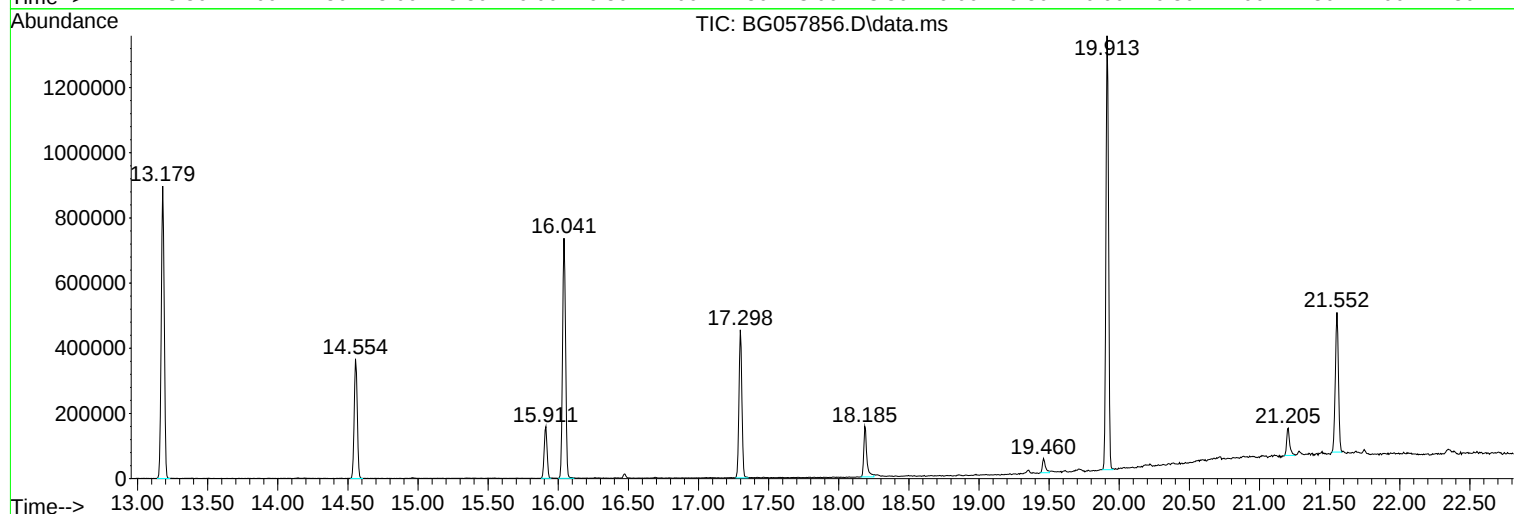
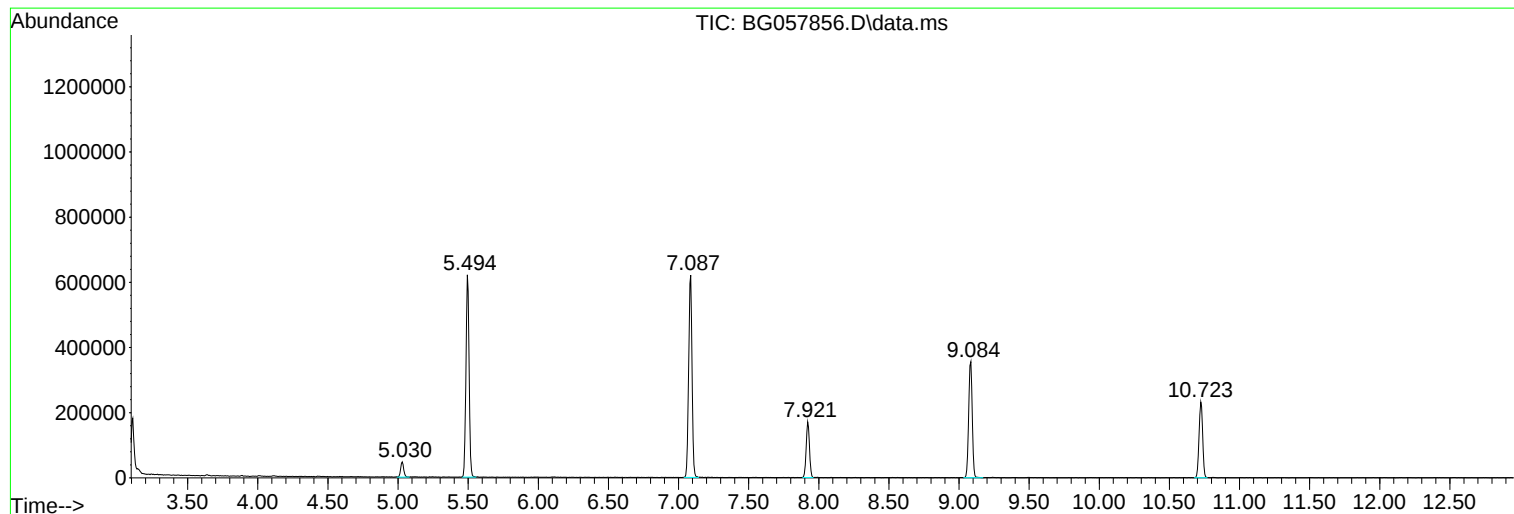
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG057856.D
Acq On : 24 Jun 2023 00:50
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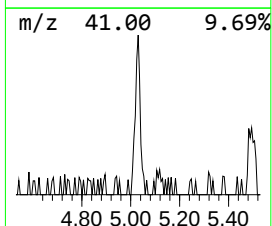
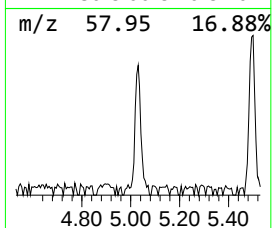
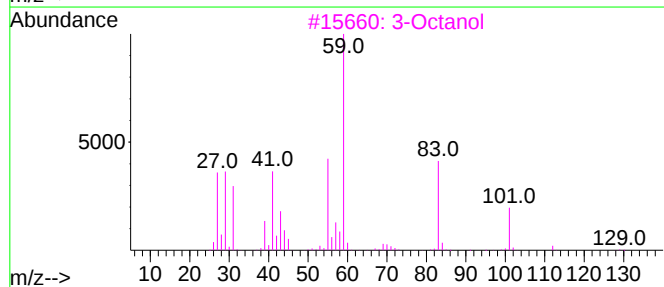
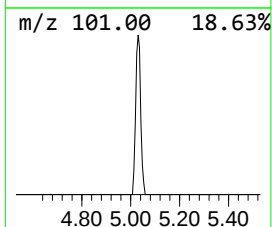
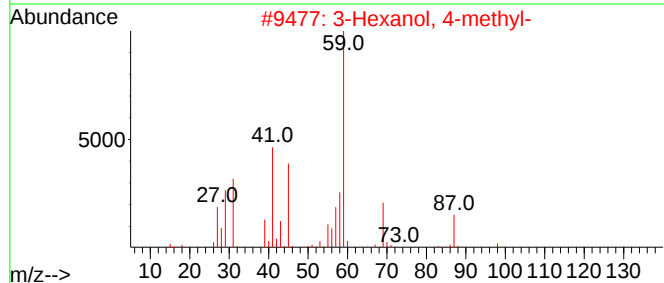
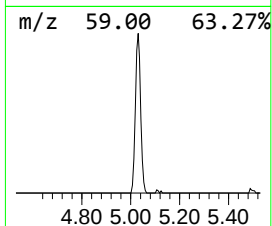
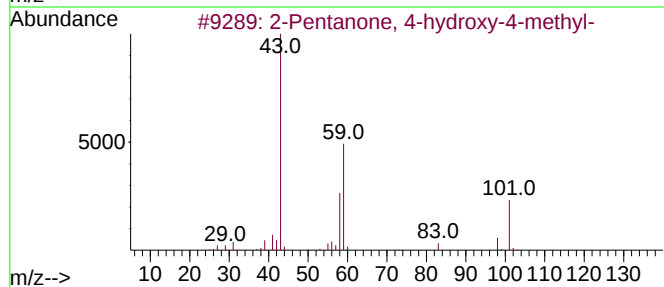
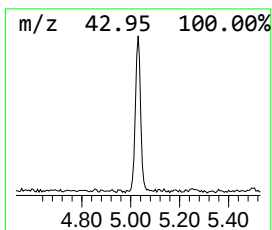
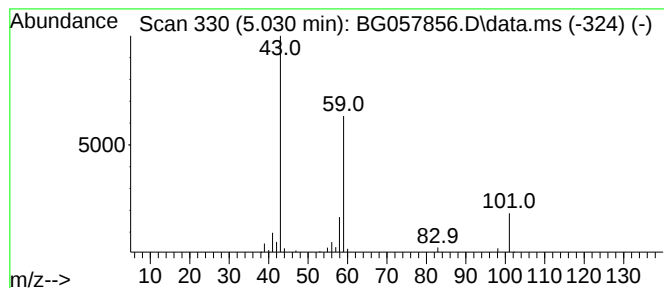
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.030	5.08 ng	71158	1,4-Dichlorobenzene-d4	7.921

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		3-Octanol	130	C8H18O	000589-98-0	33
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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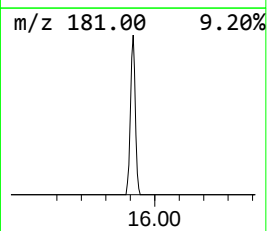
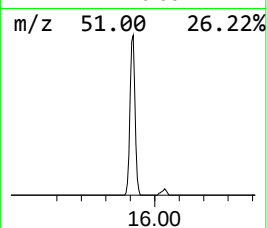
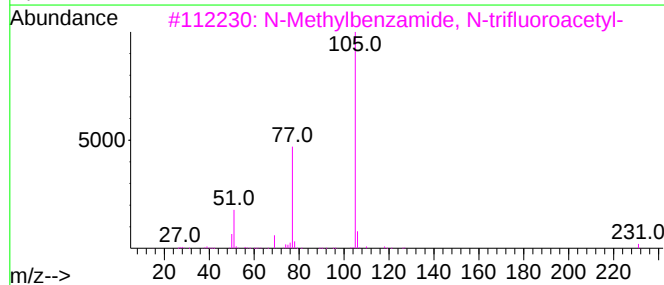
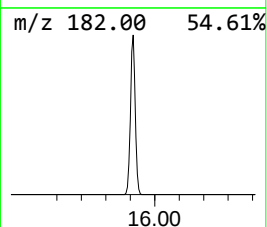
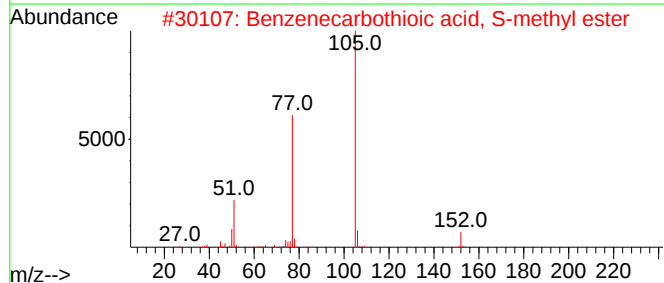
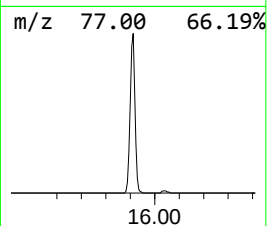
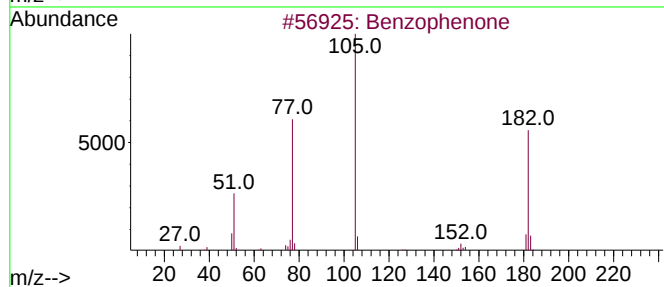
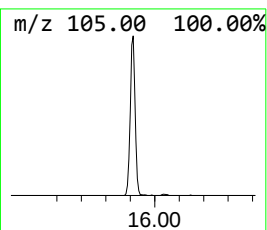
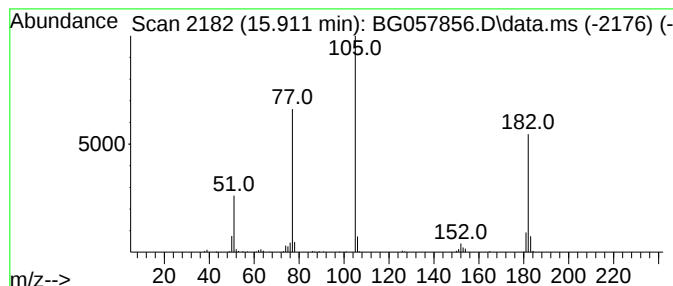
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.912	8.03 ng	221283	Acenaphthene-d10	14.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4			2-(2-Oxo-2-phenyl-ethyl)-malon...	184	C11H8N2O	1000296-76-9	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



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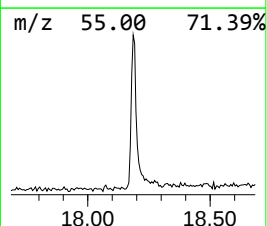
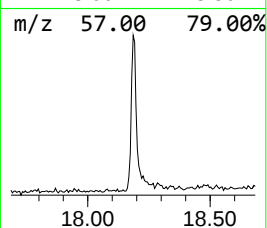
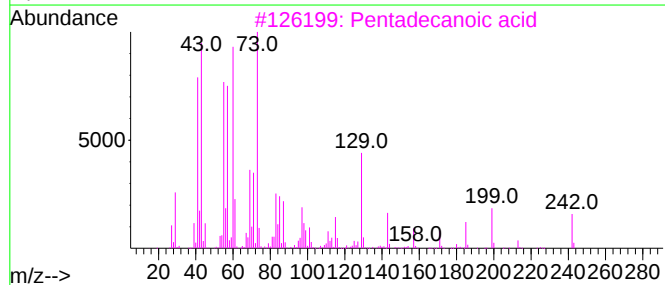
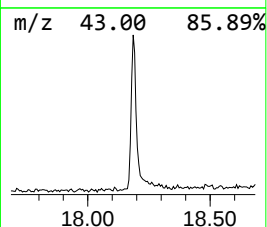
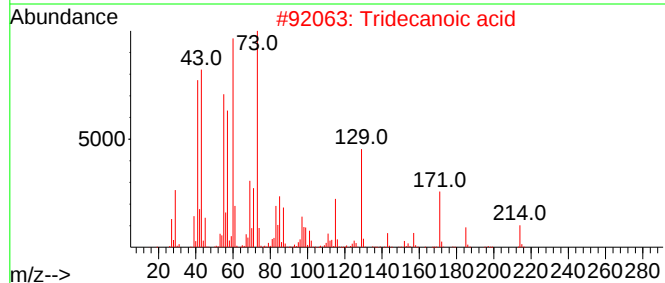
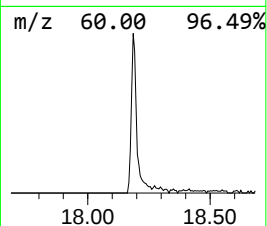
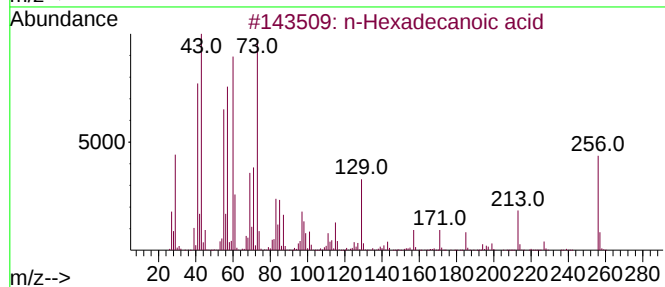
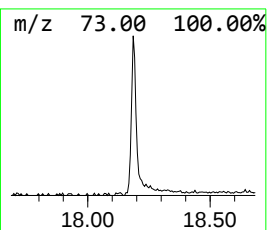
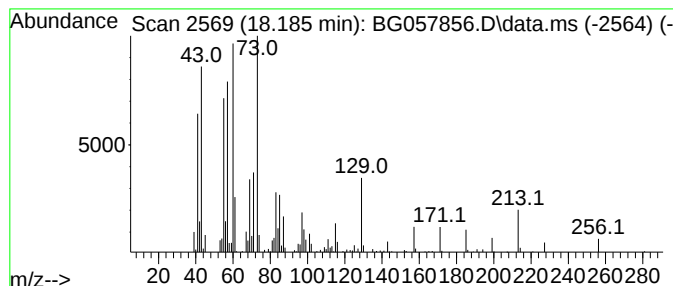
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.185	7.05 ng	233868	Phenanthrene-d10	17.298

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	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Undecanoic acid	186	C11H22O2	000112-37-8	70



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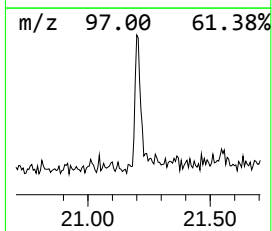
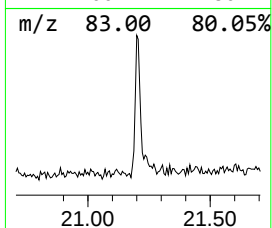
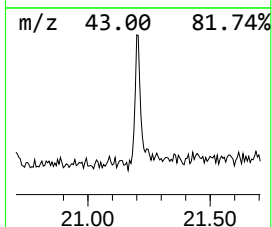
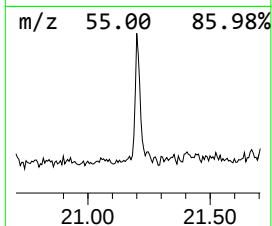
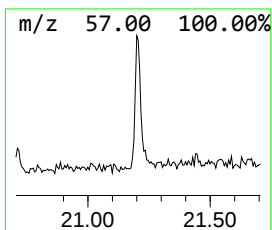
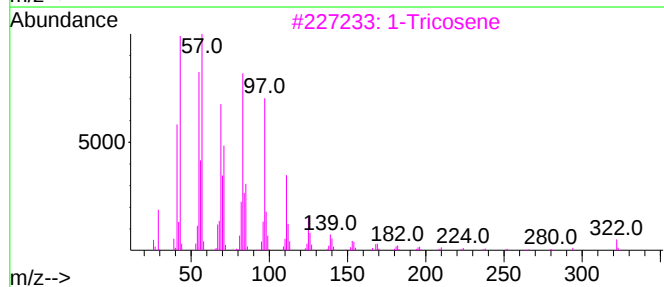
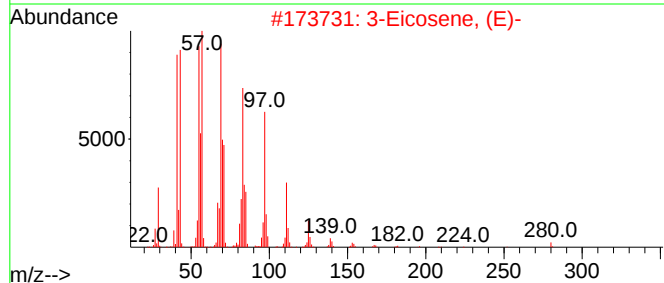
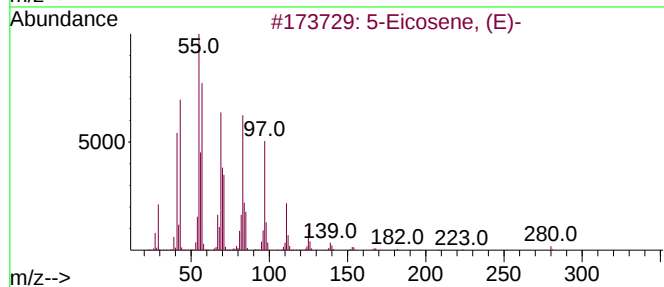
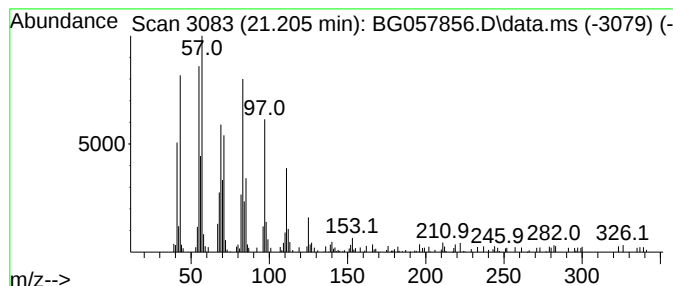
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.205	3.75 ng	125921	Chrysene-d12	21.552

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-			280	C20H40	074685-30-6	97
2	3-Eicosene, (E)-			280	C20H40	074685-33-9	95
3	1-Tricosene			322	C23H46	018835-32-0	91
4	Cyclotetracosane			336	C24H48	000297-03-0	91
5	Pentafluoropropionic acid, hexad...			388	C19H33F5O2	006222-07-7	91



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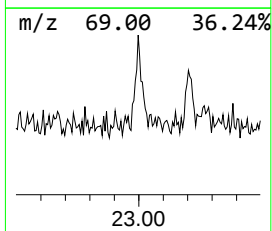
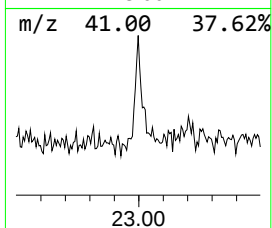
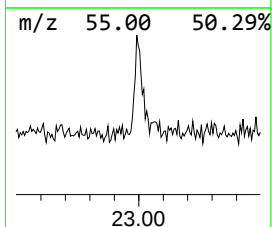
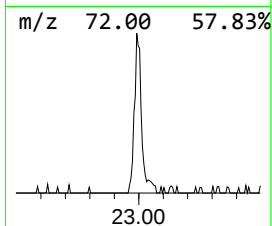
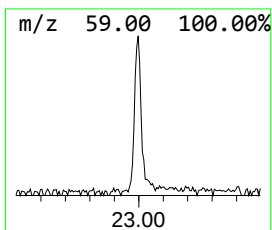
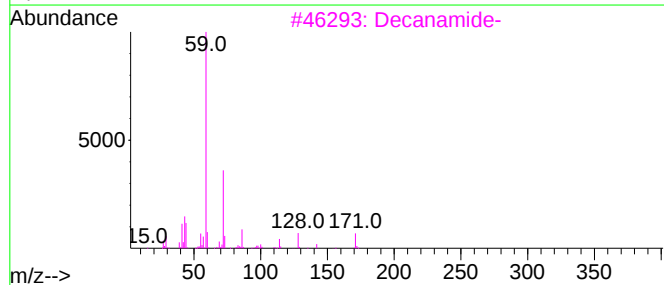
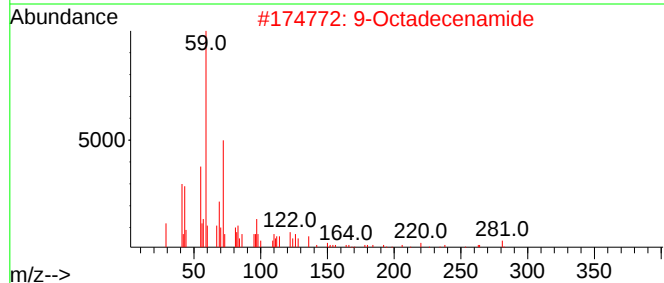
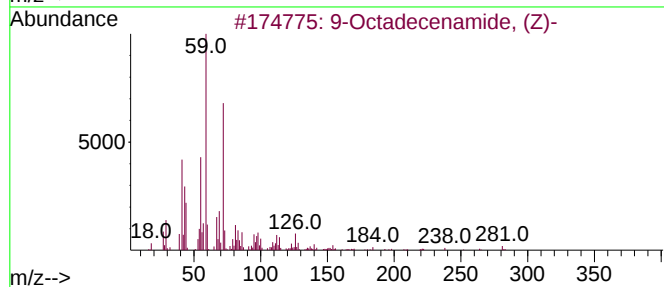
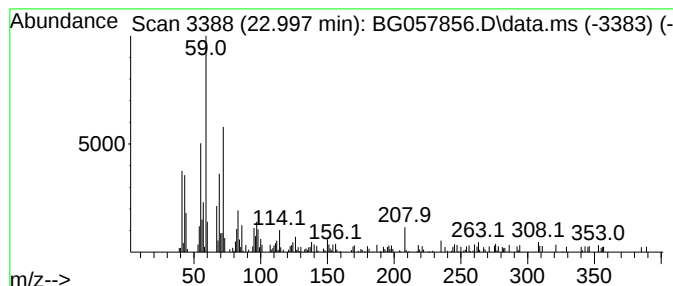
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.997	3.05 ng	102299	Chrysene-d12	21.552

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		9-Octadecenamide	281	C18H35NO	003322-62-1	64
3		Decanamide-	171	C10H21NO	002319-29-1	59
4		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	59
5		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.030	5.1	ng	71158	1	7.921	280354	20.0
Benzophenone	15.912	8.0	ng	221283	3	14.554	550917	20.0
n-Hexadecanoic ...	18.185	7.0	ng	233868	4	17.298	663748	20.0
5-Eicosene, (E)-	21.205	3.8	ng	125921	5	21.552	671611	20.0
9-Octadecenamid...	22.997	3.0	ng	102299	5	21.552	671611	20.0