

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112023\
 Data File : BG059782.D
 Acq On : 20 Nov 2023 23:51
 Operator : MA/JU
 Sample : 05378-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MH-3

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-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059782.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.827	408	415	423	rBV	433926	735078	35.81%	6.769%
2	7.454	685	692	702	rBV2	513609	922822	44.95%	8.497%
3	8.336	835	842	850	rVB2	178525	304684	14.84%	2.806%
4	9.534	1038	1046	1053	rBV2	350076	672149	32.74%	6.189%
5	11.179	1318	1326	1333	rBV	237284	447809	21.81%	4.123%
6	13.582	1728	1735	1743	rBV	984850	1496147	72.88%	13.777%
7	13.782	1762	1769	1777	rBV2	74482	131995	6.43%	1.215%
8	14.963	1963	1970	1976	rBV2	354295	557080	27.14%	5.130%
9	16.444	2216	2222	2230	rBV	843690	1282989	62.49%	11.814%
10	17.713	2431	2438	2445	rVB	452113	698812	34.04%	6.435%
11	18.524	2572	2576	2581	rBV3	99214	148307	7.22%	1.366%
12	18.947	2645	2648	2649	rBV3	21132	23332	1.14%	0.215%
13	19.663	2767	2770	2771	rBV3	24747	21757	1.06%	0.200%
14	20.286	2871	2876	2881	rVB	1649017	2052967	100.00%	18.904%
15	20.944	2985	2988	2994	rVB4	170067	217874	10.61%	2.006%
16	21.573	3093	3095	3103	rVB8	59002	85666	4.17%	0.789%
17	21.984	3163	3165	3166	rBV2	27206	22706	1.11%	0.209%
18	22.037	3169	3174	3182	rVB	329778	588704	28.68%	5.421%
19	25.627	3779	3785	3796	rVB	157927	415823	20.25%	3.829%
20	30.933	4686	4688	4690	rBV3	28202	33228	1.62%	0.306%

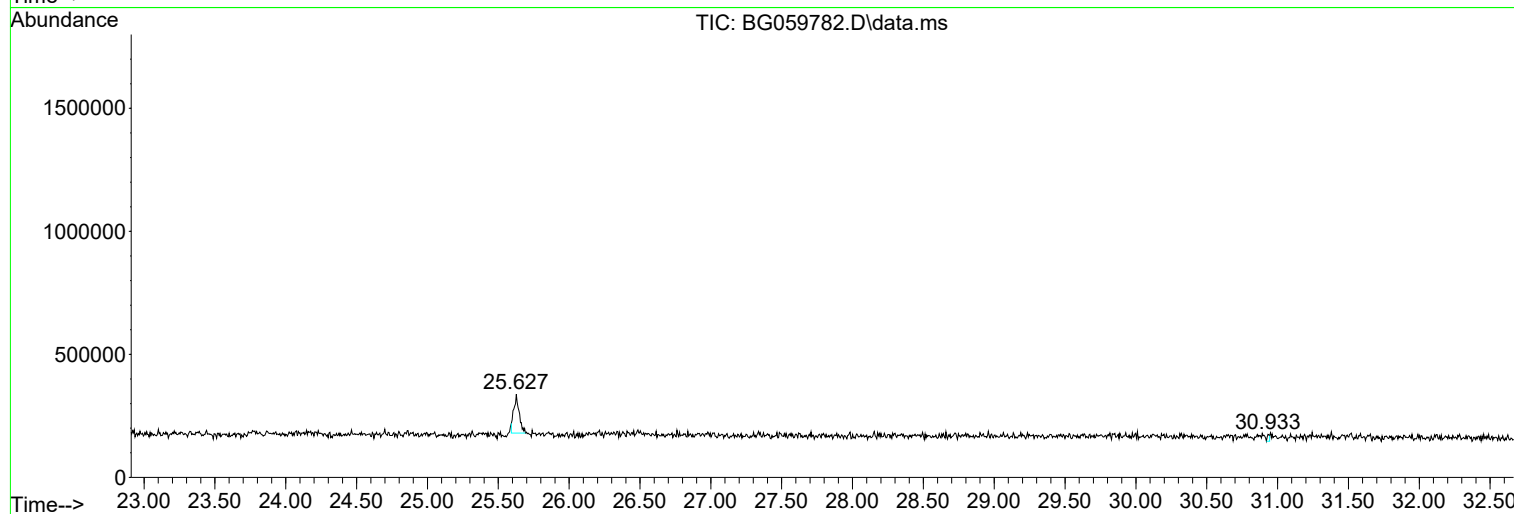
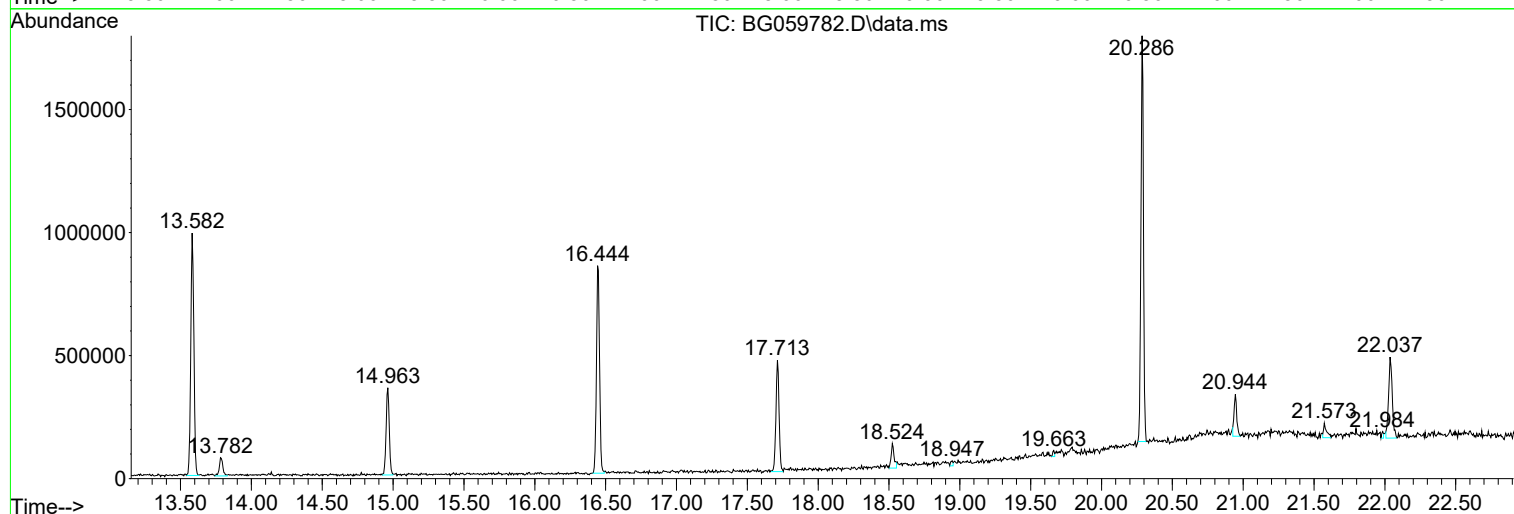
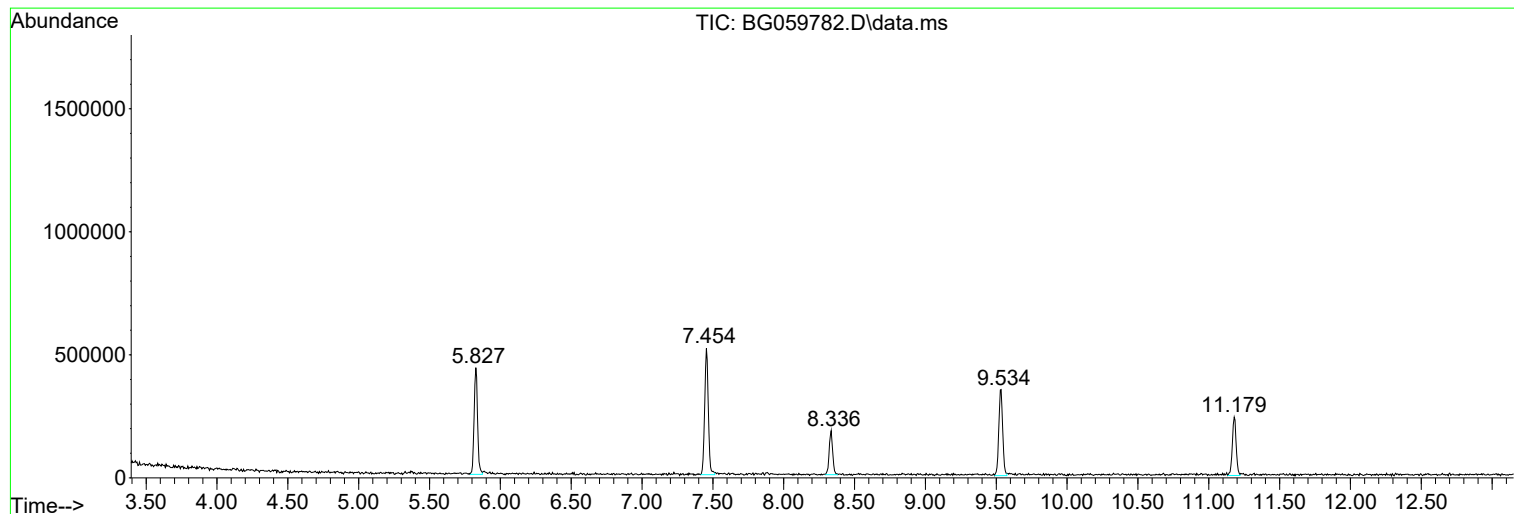
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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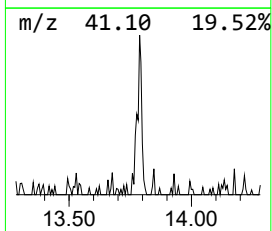
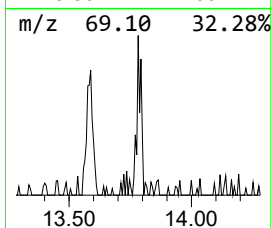
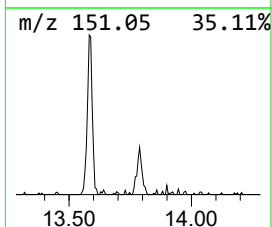
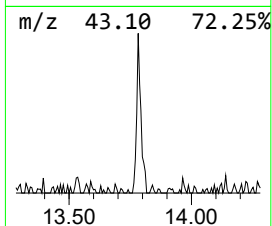
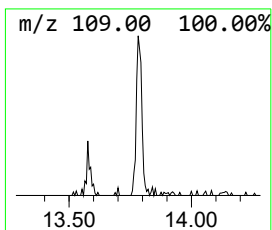
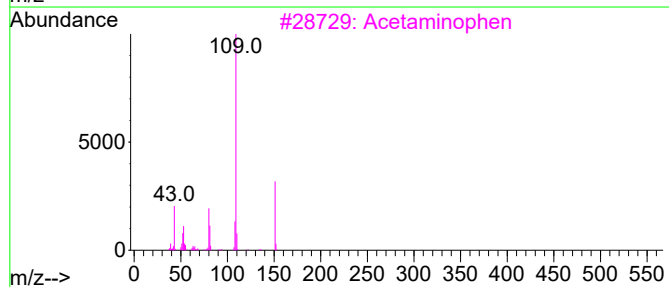
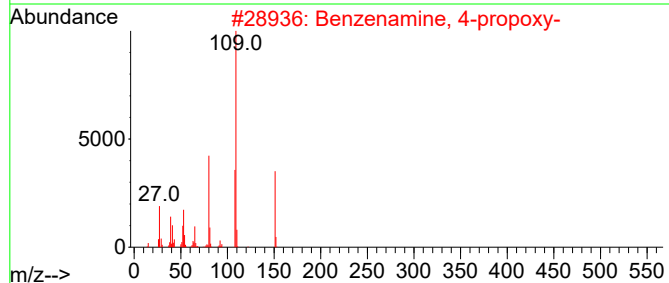
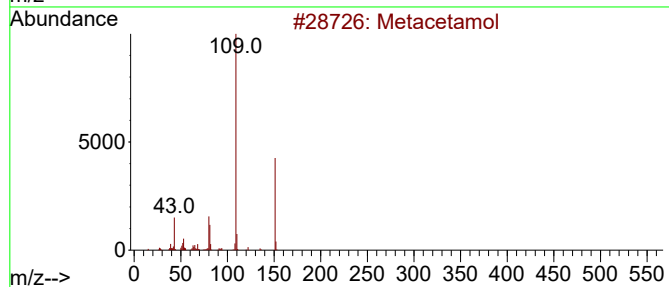
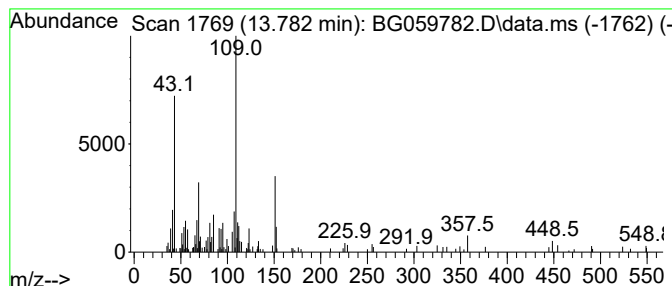
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Metacetamol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.782	4.74 ng	131995	Acenaphthene-d10	14.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Metacetamol	151	C8H9NO2	000621-42-1	72
2			Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	72
3			Acetaminophen	151	C8H9NO2	000103-90-2	64
4			2,3-Pyridinediamine	109	C5H7N3	000452-58-4	49
5			2(1H)-Pyridinone, 1-methyl-	109	C6H7NO	000694-85-9	49



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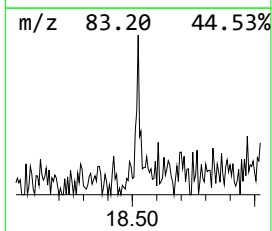
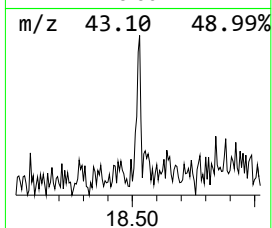
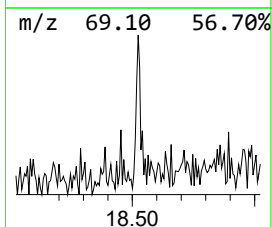
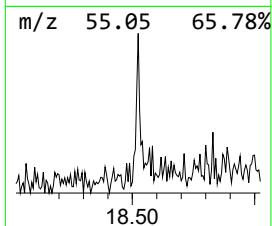
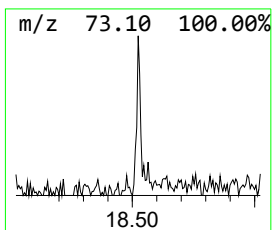
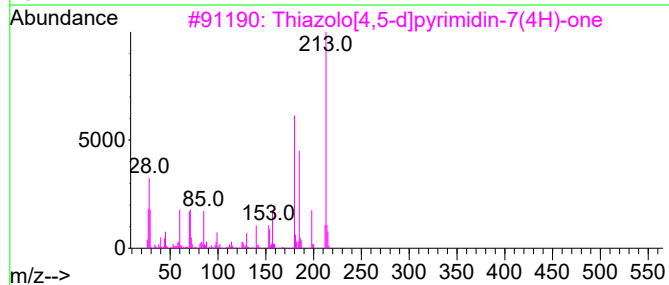
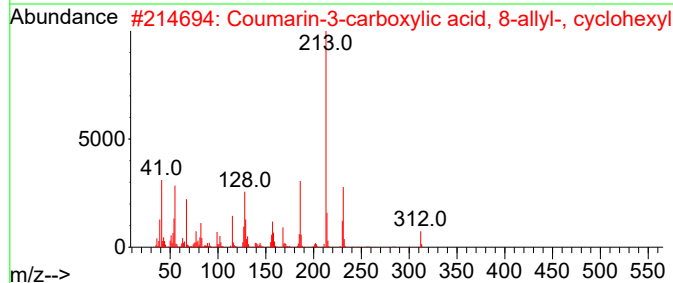
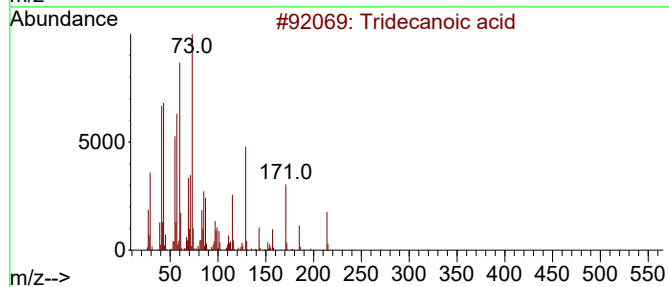
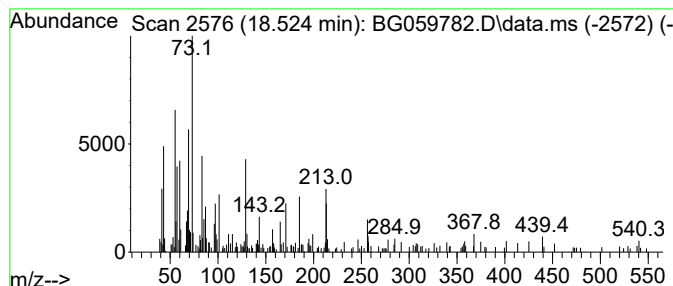
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Peak Number 2 unknown18.524 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.524	4.24 ng	148307	Phenanthrene-d10	17.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	27
2			Coumarin-3-carboxylic acid, 8-allyl-, cyclohexyl	312	C19H20O4	325472-94-4	18
3			Thiazolo[4,5-d]pyrimidin-7(4H)-one	213	C7H7N3OS2	1000153-89-3	14
4			Pyrimido[4,5-b]quinoline-2,4(1H,3H)-dione	213	C11H7N3O2	026908-38-3	11
5			10H-Phenothiazine, 10-methyl-	213	C13H11NS	001207-72-3	11



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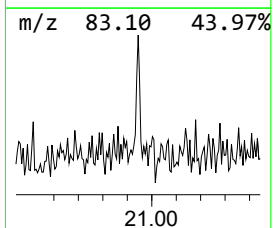
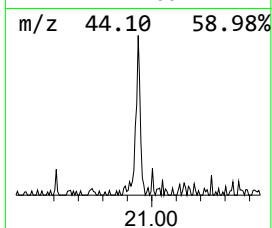
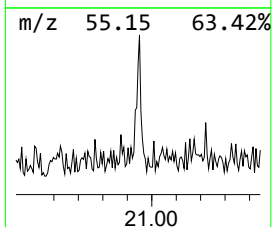
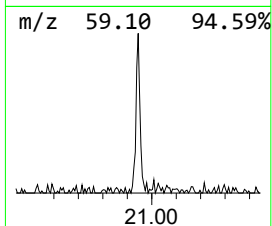
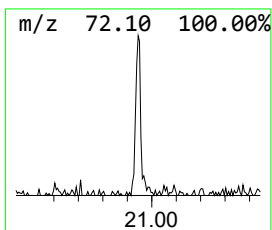
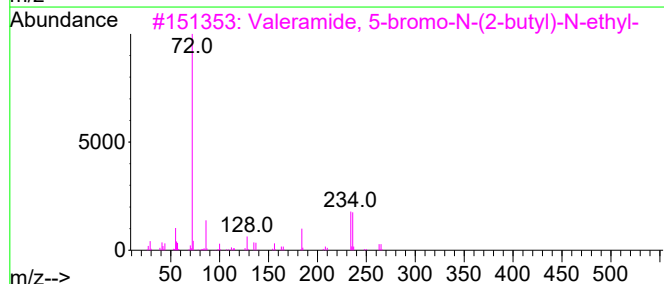
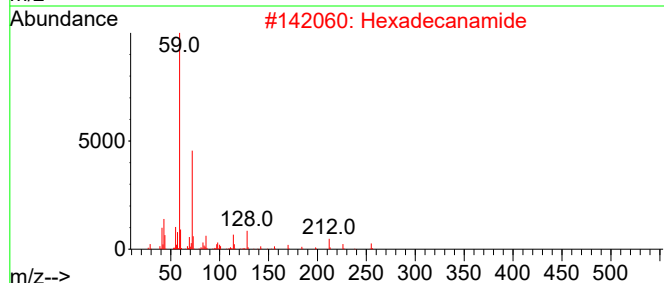
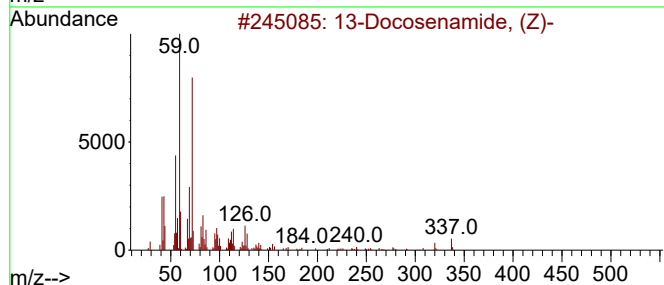
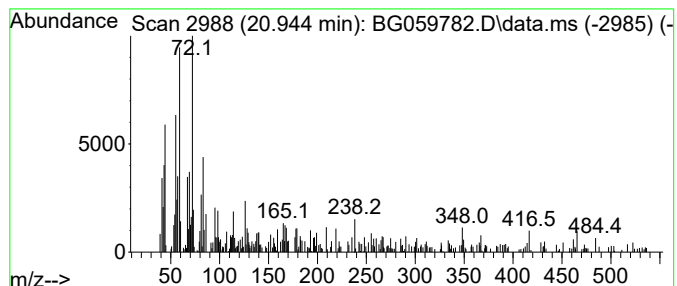
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Peak Number 3 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.944	7.40 ng	217874	Chrysene-d12	22.037

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	74
2			Hexadecanamide	255	C16H33NO	000629-54-9	42
3			Valeramide, 5-bromo-N-(2-butyl)-...	263	C11H22BrNO	1000464-14-8	38
4			Butyramide, 4-phenyl-N-propyl-N-...	317	C21H35NO	1000438-89-9	30
5			2H-Pyran, 2-ethoxy-3,4-dihydro-	128	C7H12O2	000103-75-3	30



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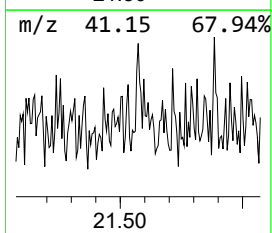
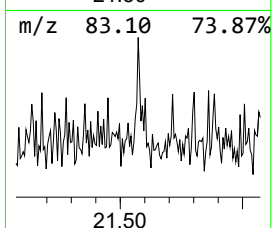
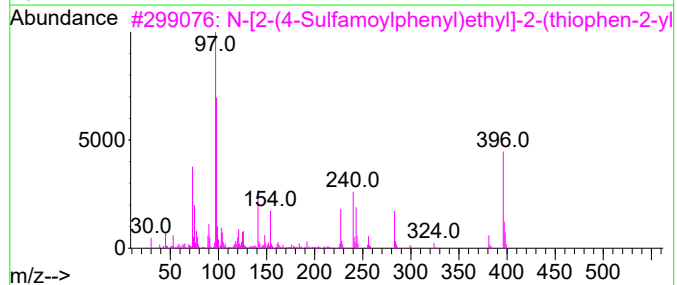
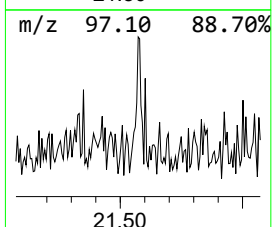
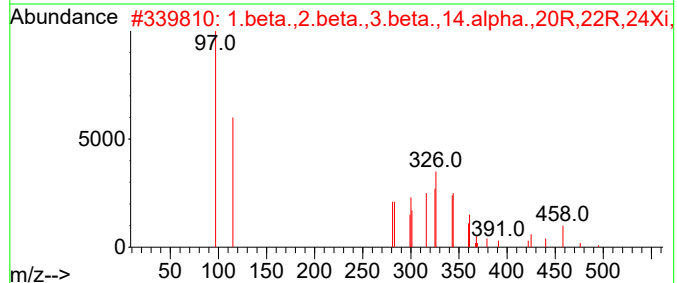
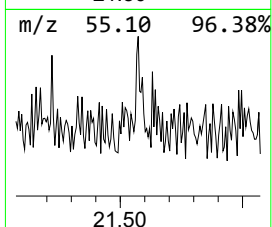
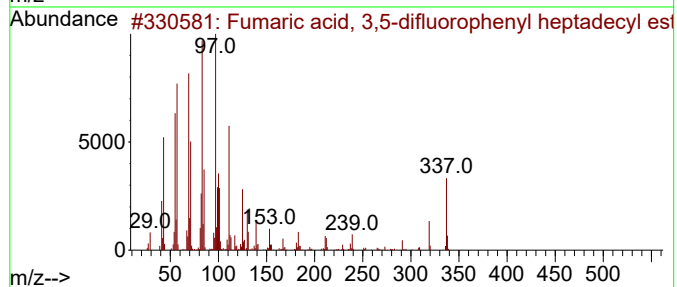
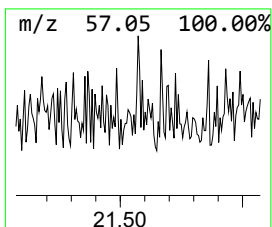
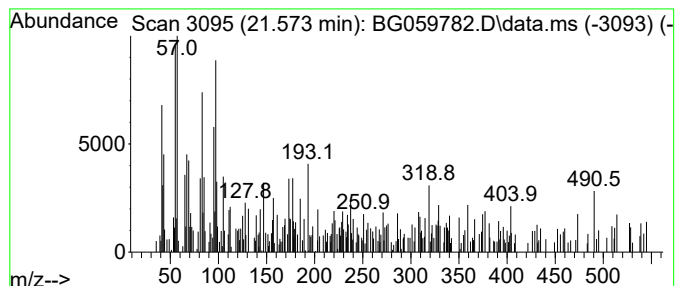
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Peak Number 4 unknown21.573 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.573	2.91 ng	85666	Chrysene-d12	22.037

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fumaric acid, 3,5-difluorophenyl...	466	C27H40F2O4	1000339-38-2	16
2			1.beta.,2.beta.,3.beta.,14.alpha...	512	C27H44O9	102099-20-7	12
3			N-[2-(4-Sulfamoylphenyl)ethyl]-2...	396	C17H24N2O3S2Si	1000512-06-5	12
4			2-(1,3-Benzothiazol-2-yl)-4-[(2...	408	C17H11F3N4O5S2	328280-06-4	9
5			Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Metacetamol	13.782	4.7	ng	131995	3	14.963	557080	20.0
unknown18.524	18.524	4.2	ng	148307	4	17.713	698812	20.0
13-Docosenamide...	20.944	7.4	ng	217874	5	22.037	588704	20.0
unknown21.573	21.573	2.9	ng	85666	5	22.037	588704	20.0