

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112223\
 Data File : BG059822.D
 Acq On : 22 Nov 2023 17:40
 Operator : MA/JU
 Sample : 05449-10
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-SED-04

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: BG059822.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.367	331	337	343	rBV2	197268	292348	14.12%	3.234%
2	5.826	408	415	422	rBV2	205619	330718	15.97%	3.659%
3	7.453	683	692	700	rBV2	284723	522169	25.21%	5.777%
4	8.329	833	841	850	rBV2	103946	195403	9.44%	2.162%
5	9.533	1037	1046	1055	rBV2	190537	337180	16.28%	3.730%
6	11.178	1320	1326	1335	rVB	130334	238293	11.51%	2.636%
7	13.581	1728	1735	1741	rBV	827949	1299076	62.73%	14.372%
8	13.787	1765	1770	1778	rVB3	152200	252747	12.20%	2.796%
9	14.328	1858	1862	1865	rBV5	18073	23640	1.14%	0.262%
10	14.868	1951	1954	1958	rBV5	19543	27683	1.34%	0.306%
11	14.962	1962	1970	1976	rVV	314856	510501	24.65%	5.648%
12	15.150	1997	2002	2008	rVB7	28737	46368	2.24%	0.513%
13	16.449	2215	2223	2229	rBV3	392099	610688	29.49%	6.756%
14	17.712	2433	2438	2444	rBV	390832	598505	28.90%	6.621%
15	18.129	2502	2509	2512	rBV7	13323	29303	1.41%	0.324%
16	18.523	2572	2576	2580	rBV5	48947	77192	3.73%	0.854%
17	19.463	2733	2736	2739	rBV5	22895	32315	1.56%	0.358%
18	19.592	2755	2758	2760	rBV4	17184	23989	1.16%	0.265%
19	19.745	2781	2784	2787	rVB5	23874	25448	1.23%	0.282%
20	19.792	2787	2792	2793	rBV5	40367	41830	2.02%	0.463%
21	19.903	2809	2811	2814	rBV4	17948	21571	1.04%	0.239%
22	19.986	2823	2825	2829	rVV5	20750	28343	1.37%	0.314%
23	20.109	2843	2846	2850	rVB6	25743	34854	1.68%	0.386%
24	20.238	2864	2868	2869	rBV4	15678	21483	1.04%	0.238%
25	20.291	2871	2877	2884	rVB	1557640	2071037	100.00%	22.912%
26	21.031	3002	3003	3008	rBV5	27784	22009	1.06%	0.243%
27	21.572	3091	3095	3102	rBV10	33357	65528	3.16%	0.725%
28	22.042	3169	3175	3182	rVB	341455	548514	26.48%	6.068%
29	23.440	3412	3413	3417	rBV3	21299	24590	1.19%	0.272%
30	24.545	3599	3601	3606	rVB6	15991	24233	1.17%	0.268%
31	25.620	3775	3784	3797	rBV3	183940	609565	29.43%	6.744%
32	31.055	4706	4709	4711	rVB4	20434	26076	1.26%	0.288%
33	31.084	4711	4714	4717	rBV5	19975	25826	1.25%	0.286%

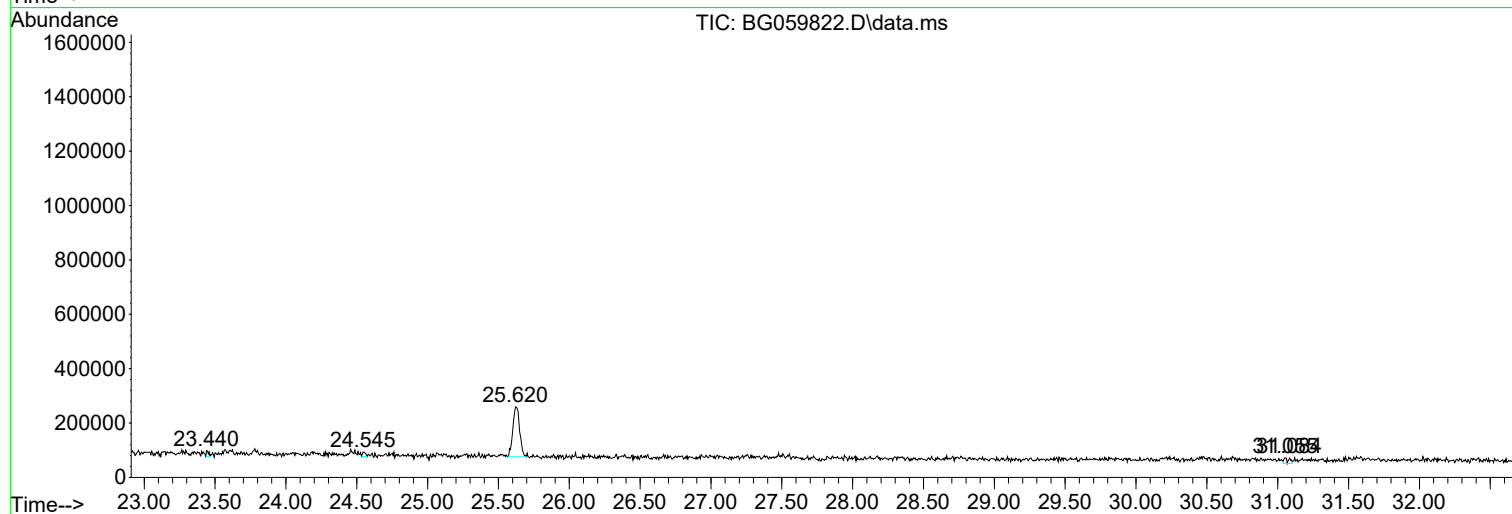
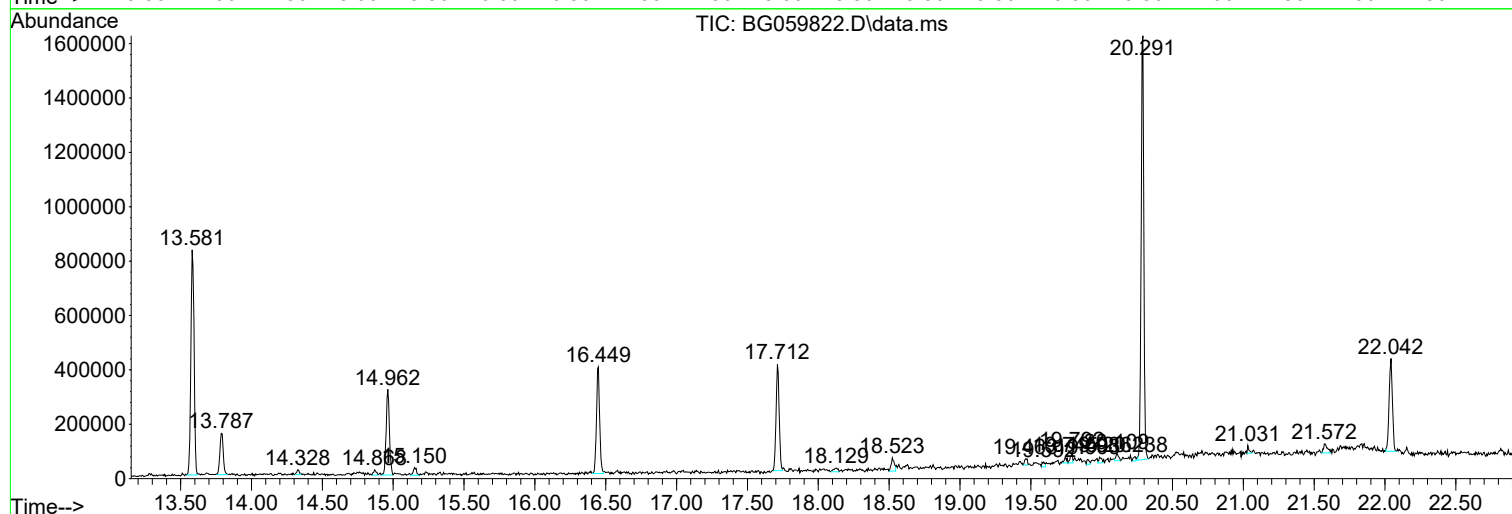
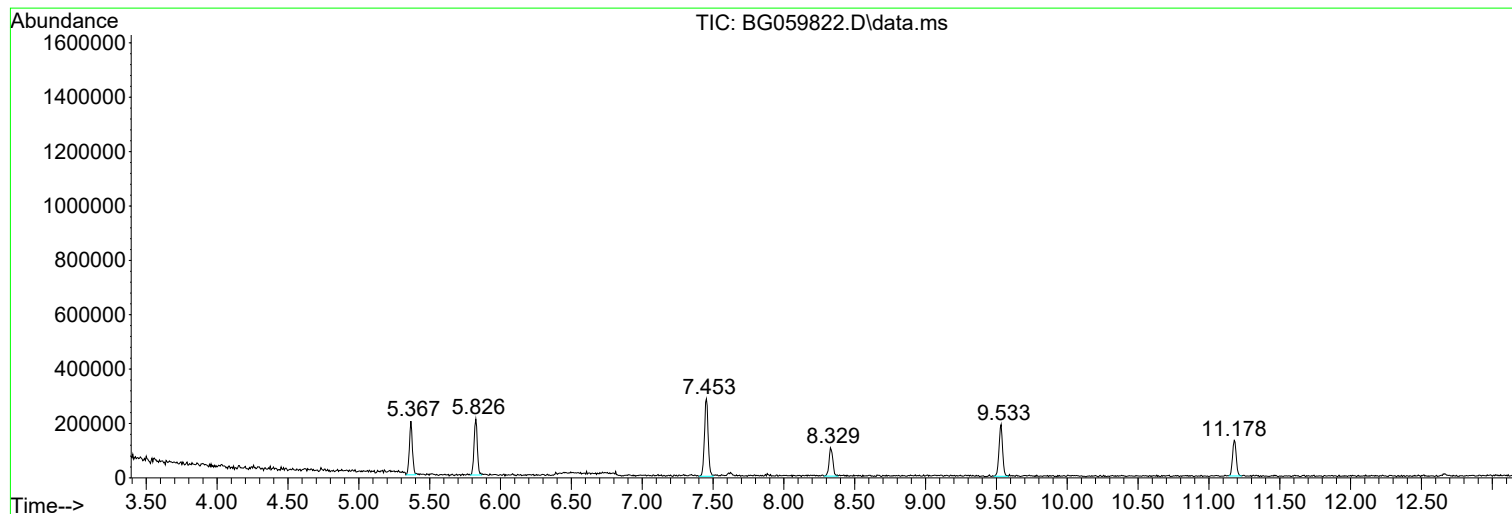
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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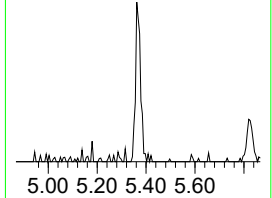
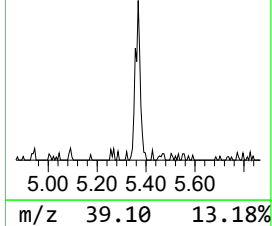
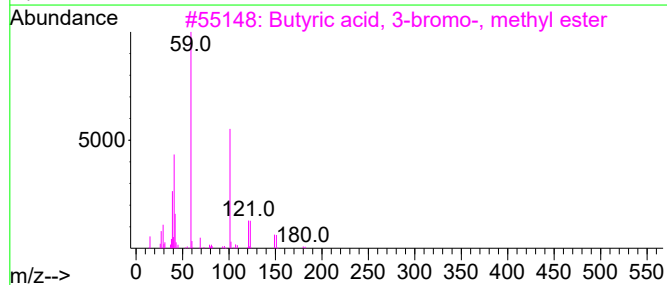
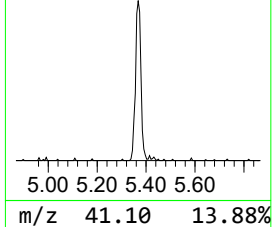
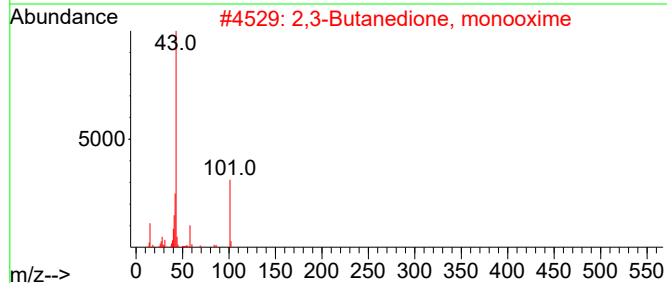
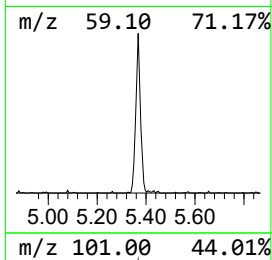
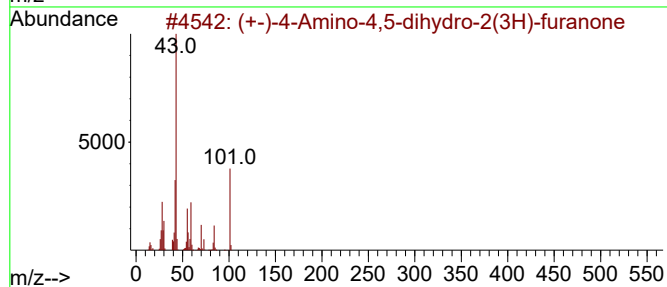
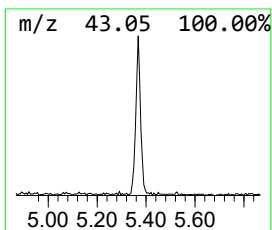
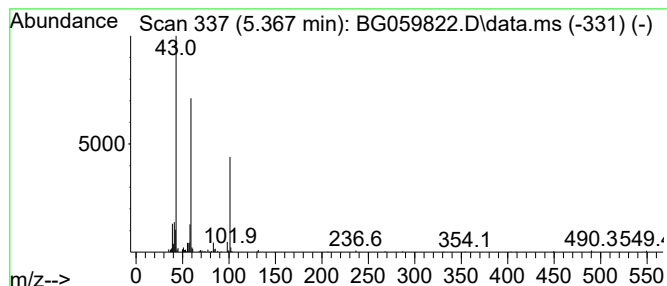
Instrument :
BNA_G
ClientSampleId :
WC-SED-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG11623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (+)-4-Amino-4,5-dihydro-2(... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.367	29.92 ng	292348	1,4-Dichlorobenzene-d4		8.329	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...		101	C4H7NO2	016504-58-8	50
2	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	46
3	Butyric acid, 3-bromo-, methyl e...		180	C5H9BrO2	021249-59-2	38
4	Butanoic acid, 4-iodo-, methyl e...		228	C5H9IO2	014273-85-9	38
5	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	38



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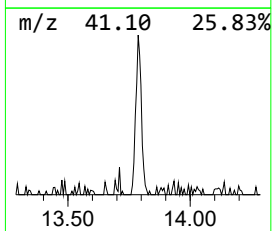
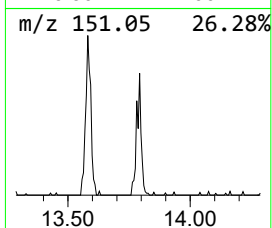
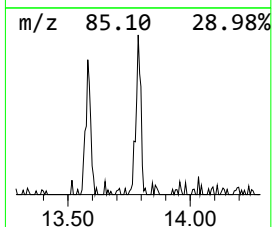
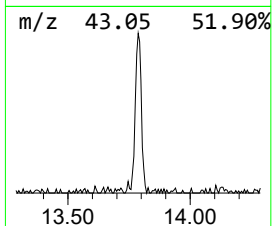
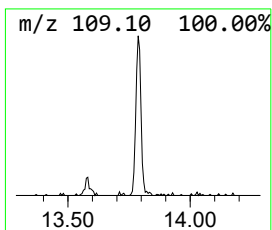
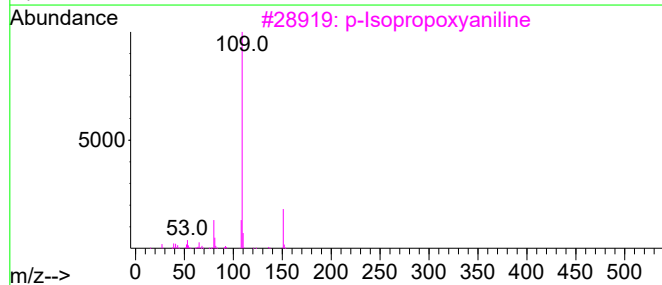
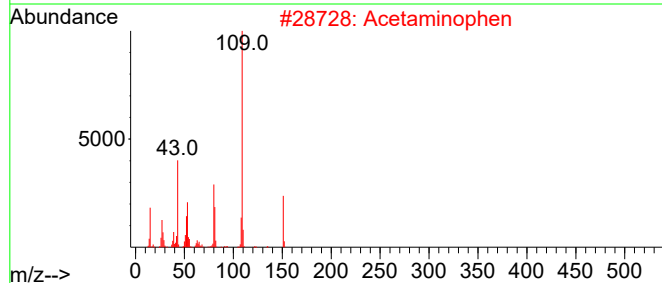
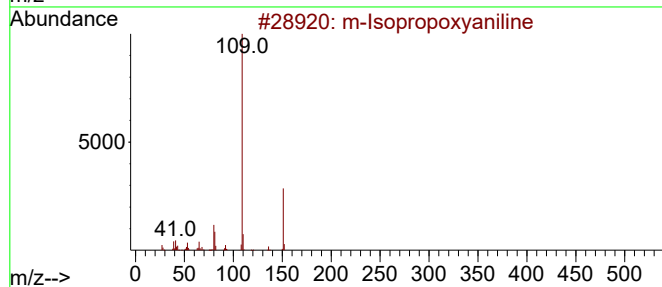
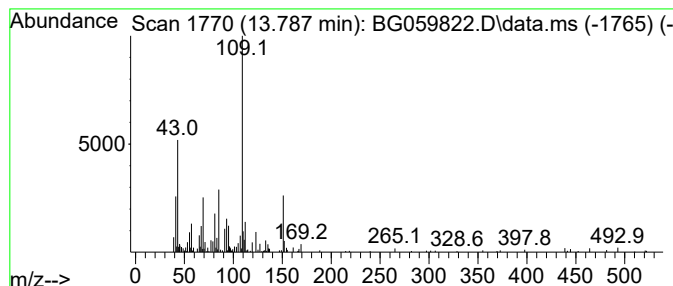
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 m-Isopropoxyaniline Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.787	9.90 ng	252747	Acenaphthene-d10	14.956

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	58
2			Acetaminophen	151	C8H9NO2	000103-90-2	53
3			p-Isopropoxyaniline	151	C9H13NO	007664-66-6	53
4			4-Pyridinemethanol, acetate (ester)	151	C8H9NO2	001007-48-3	53
5			Metacetamol	151	C8H9NO2	000621-42-1	53



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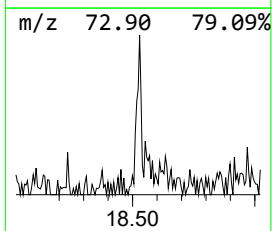
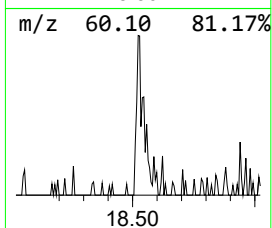
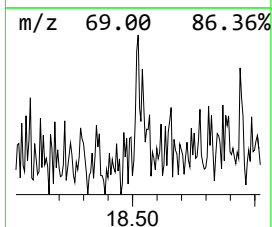
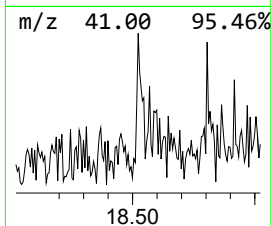
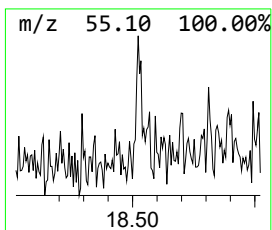
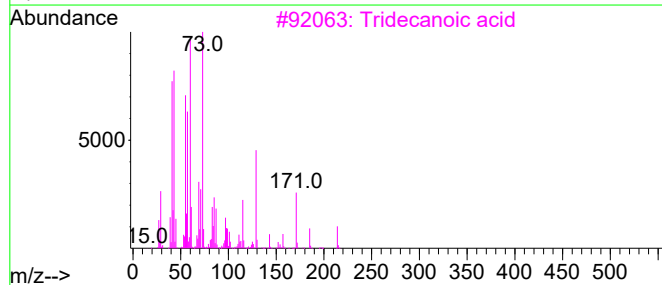
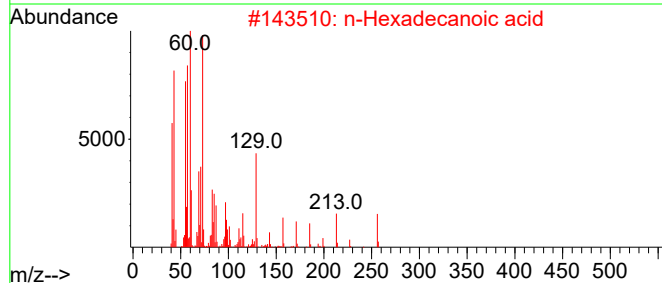
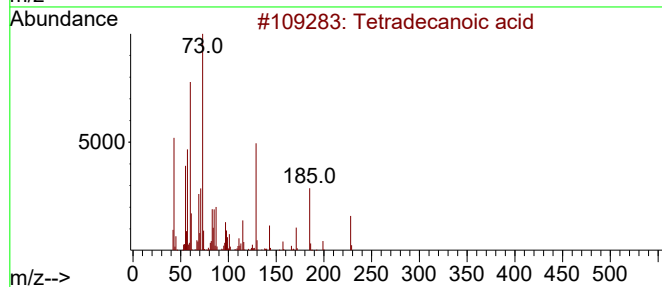
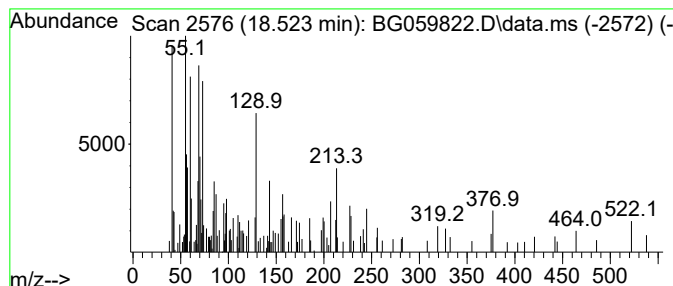
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown18.523 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.523	2.58 ng	77192	Phenanthrene-d10	17.712

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	38
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	30
3			Tridecanoic acid	214	C13H26O2	000638-53-9	25
4			Dodecanoic acid	200	C12H24O2	000143-07-7	25
5			Undecanoic acid	186	C11H22O2	000112-37-8	18



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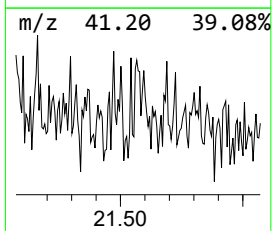
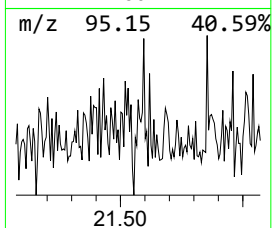
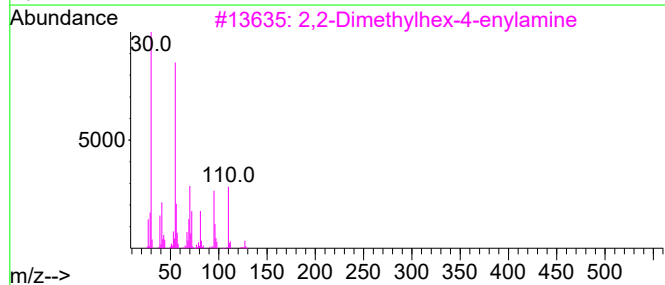
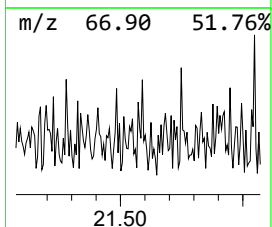
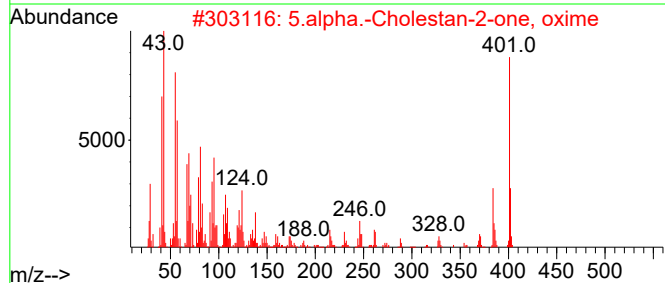
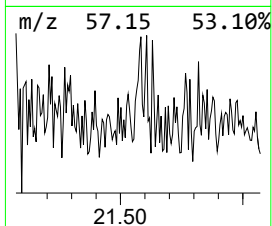
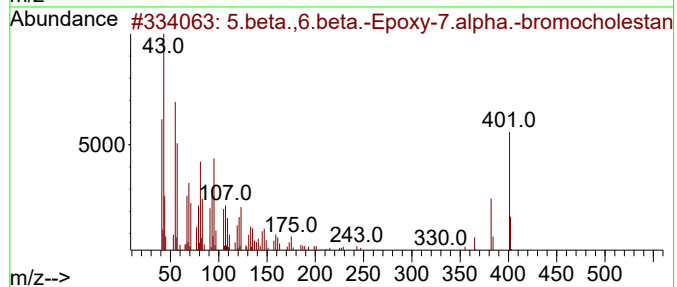
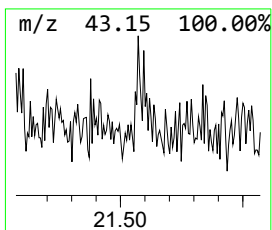
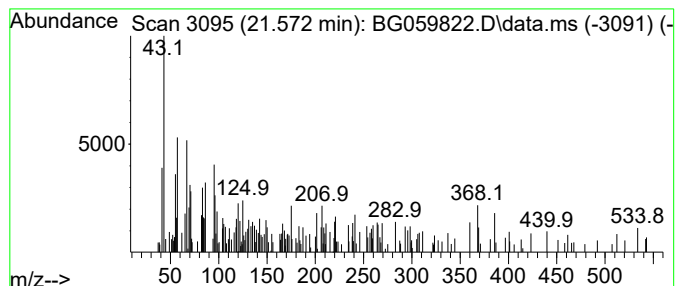
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown21.572 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.572	2.39 ng	65528	Chrysene-d12	22.042

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5.beta.,6.beta.-Epoxy-7.alpha.-b...	480	C27H45BrO2	095841-70-6	16		
2	5.alpha.-Cholestan-2-one, oxime	401	C27H47NO	014614-13-2	12		
3	2,2-Dimethylhex-4-enylamine	127	C8H17N	133885-74-2	12		
4	Cholesteryl 3-cyclohexylbutyrate	538	C37H62O2	1000252-82-2	10		
5	7-Dehydrocholesterol isocaproate	484	C33H56O2	1000252-60-9	10		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(+)-4-Amino-4,...	5.367	29.9	ng	292348	1	8.329	195403	20.0
m-Isopropoxyani...	13.787	9.9	ng	252747	3	14.956	510501	20.0
unknown18.523	18.523	2.6	ng	77192	4	17.712	598505	20.0
unknown21.572	21.572	2.4	ng	65528	5	22.042	548514	20.0