

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032423\
 Data File : BM039154.D
 Acq On : 24 Mar 2023 22:51
 Operator : CG/JU
 Sample : 02049-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 OK-02-032323

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-BM030823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039154.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.428	189	194	199	rBV	61487	78131	1.07%	0.162%
2	5.040	290	298	307	rBV	1145012	1563673	21.50%	3.251%
3	5.504	371	377	389	rVB	2738281	3893586	53.53%	8.094%
4	7.116	640	651	665	rBV	2657201	4109756	56.50%	8.543%
5	7.951	784	793	800	rVB	934248	1488402	20.46%	3.094%
6	9.116	984	991	999	rBV	1614552	2584363	35.53%	5.372%
7	10.763	1259	1271	1279	rBV	1236345	2148173	29.53%	4.466%
8	13.216	1681	1688	1698	rBV	3704337	5501783	75.63%	11.437%
9	14.316	1870	1875	1881	rBV	46250	81382	1.12%	0.169%
10	14.592	1912	1922	1929	rBV	1795211	2604529	35.80%	5.414%
11	15.433	2061	2065	2069	rVB	74414	88407	1.22%	0.184%
12	15.839	2124	2134	2139	rBV	50777	126529	1.74%	0.263%
13	15.951	2147	2153	2158	rBV	477972	646913	8.89%	1.345%
14	16.080	2168	2175	2182	rBV	3082357	4341202	59.68%	9.024%
15	16.298	2207	2212	2214	rBV	145213	205679	2.83%	0.428%
16	16.874	2306	2310	2317	rBV	203450	264715	3.64%	0.550%
17	17.086	2343	2346	2350	rBV	191662	229145	3.15%	0.476%
18	17.145	2352	2356	2360	rVB	89941	123967	1.70%	0.258%
19	17.339	2383	2389	2394	rBV	2101771	2929599	40.27%	6.090%
20	17.380	2394	2396	2402	rVB	94252	134545	1.85%	0.280%
21	17.827	2469	2472	2477	rBV	200917	241013	3.31%	0.501%
22	18.004	2499	2502	2507	rVB	133572	157500	2.17%	0.327%
23	18.233	2536	2541	2551	rBV2	613663	1107677	15.23%	2.303%
24	18.339	2557	2559	2563	rBV2	92509	101883	1.40%	0.212%
25	18.521	2587	2590	2594	rBV	197623	232832	3.20%	0.484%
26	19.151	2693	2697	2700	rBV2	322759	458640	6.30%	0.953%
27	19.956	2830	2834	2844	rVB	5860506	7274248	100.00%	15.122%
28	21.515	3096	3099	3104	rVB	2123825	2757383	37.91%	5.732%
29	23.944	3509	3512	3520	rVB2	1422833	2629664	36.15%	5.466%

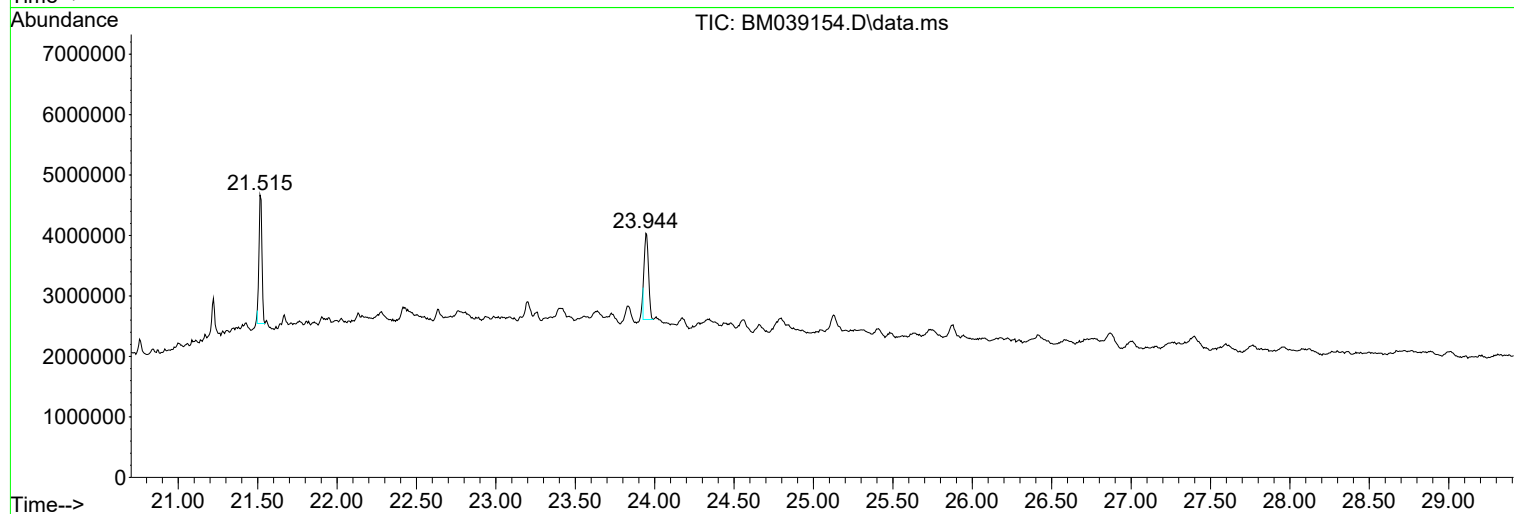
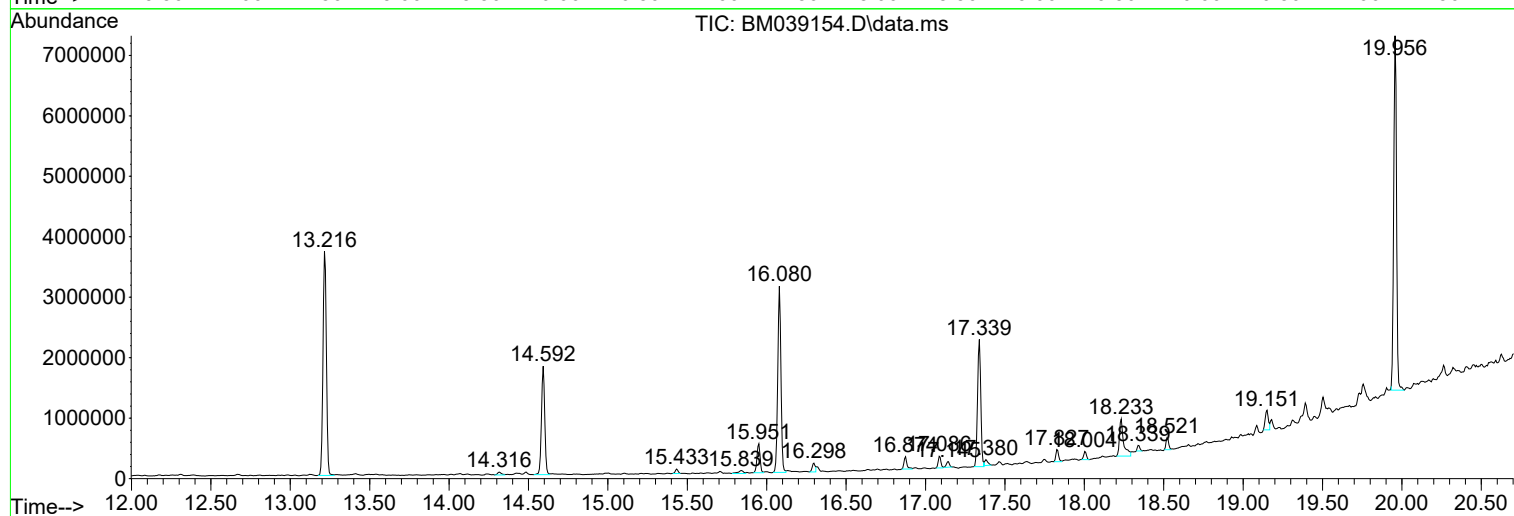
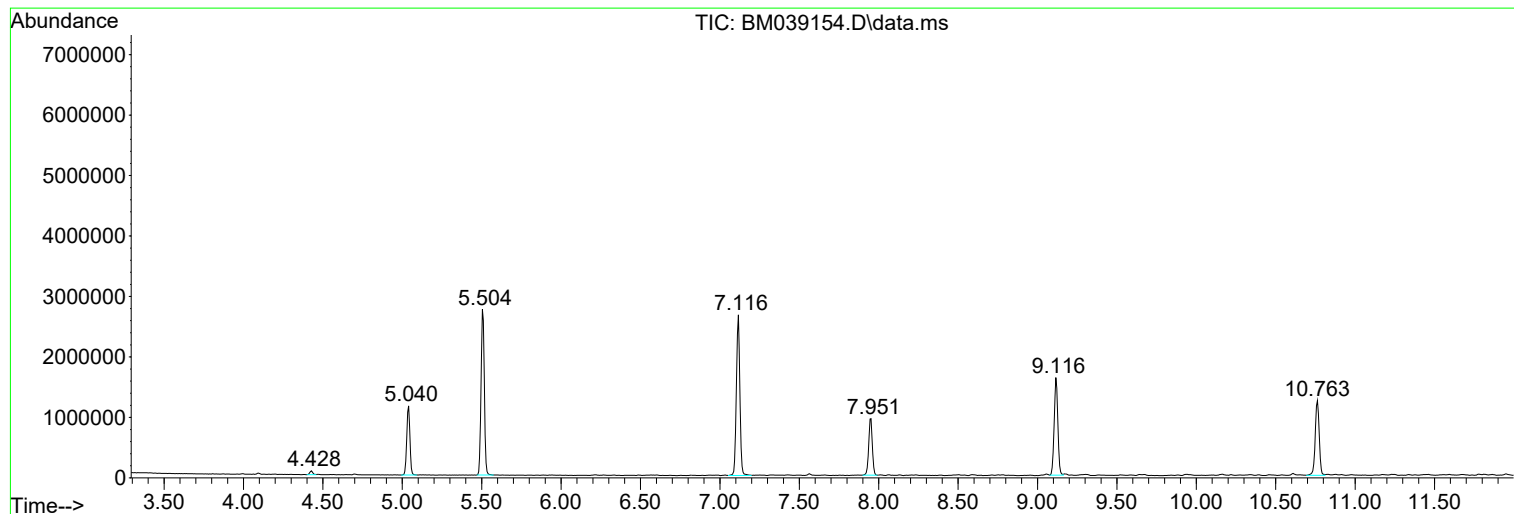
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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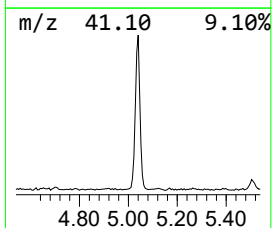
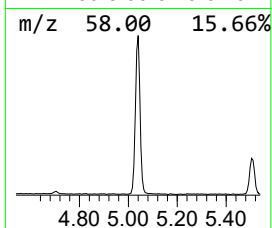
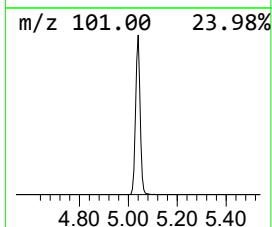
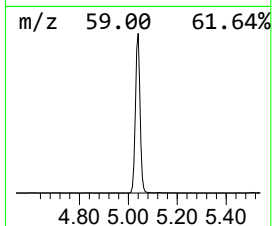
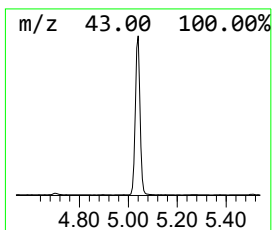
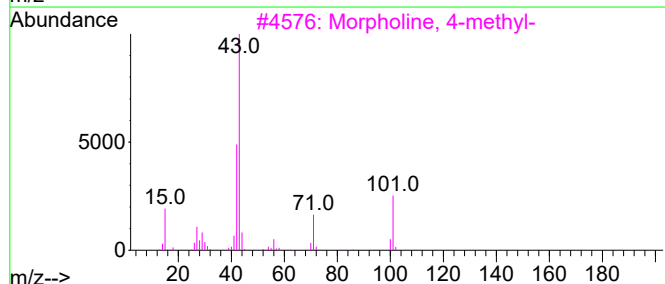
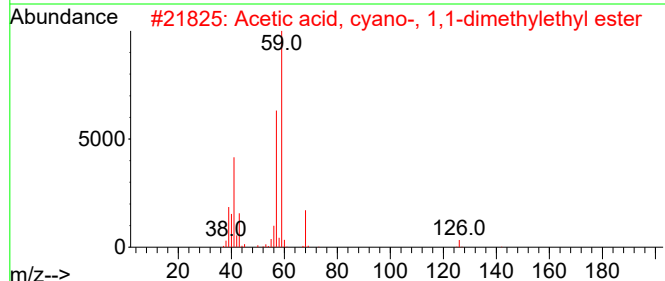
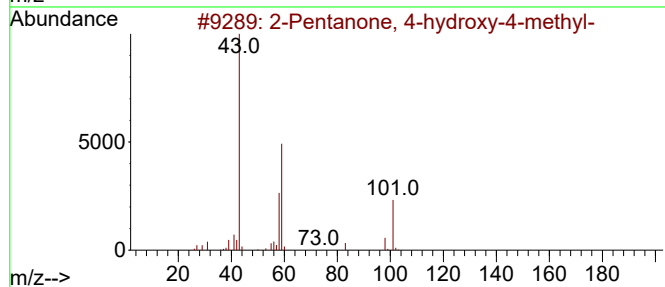
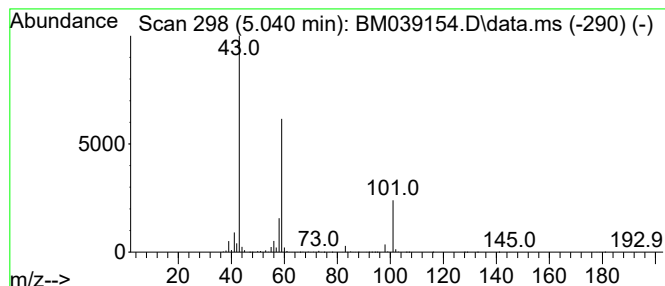
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM030823.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	21.01 ng	1563670	1,4-Dichlorobenzene-d4	7.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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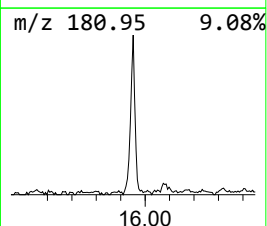
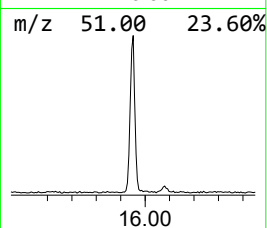
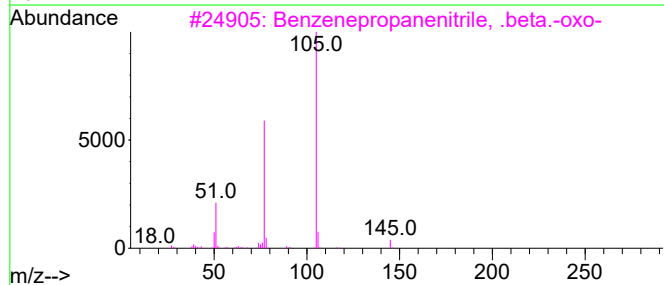
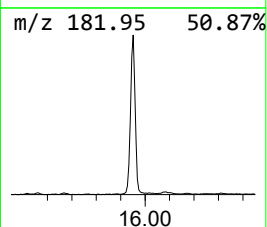
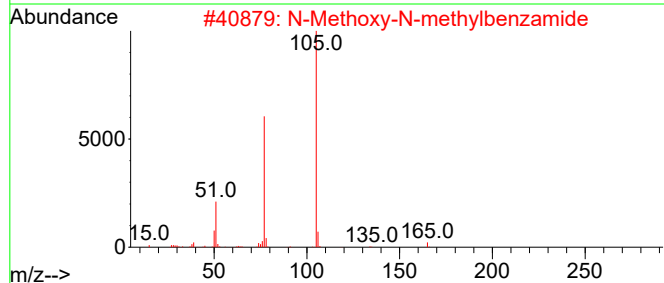
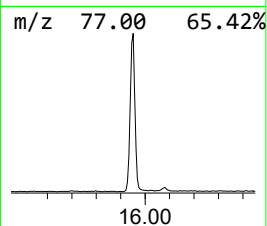
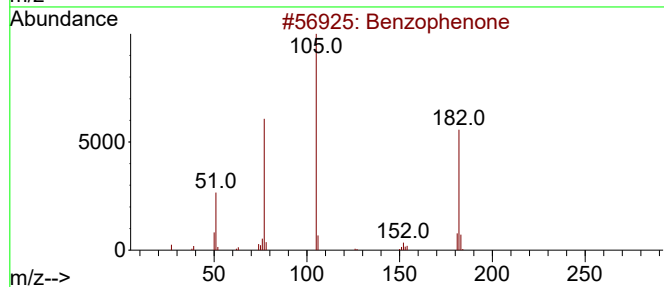
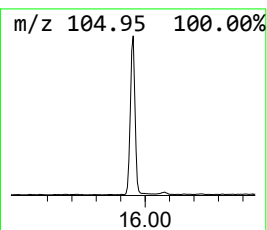
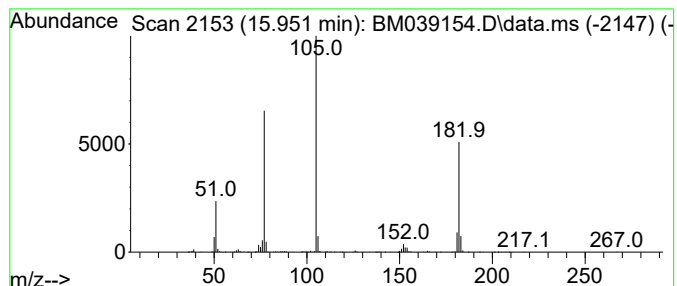
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	4.97 ng	646913	Acenaphthene-d10	14.592

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
3			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	47



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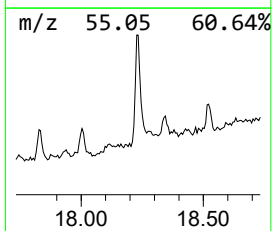
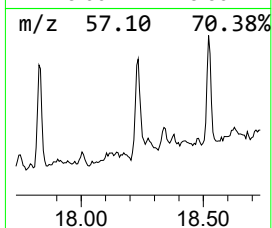
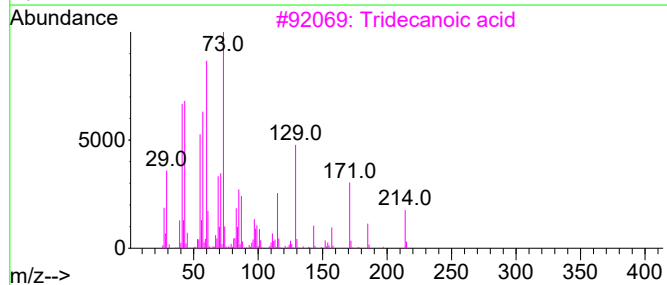
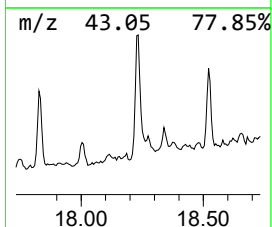
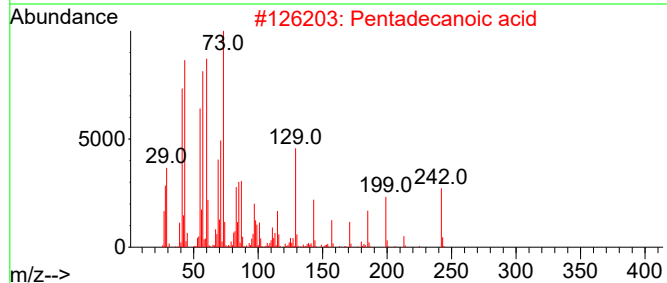
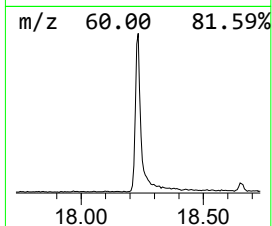
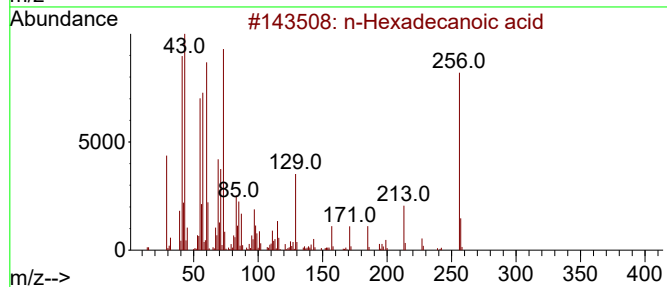
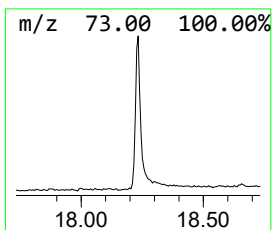
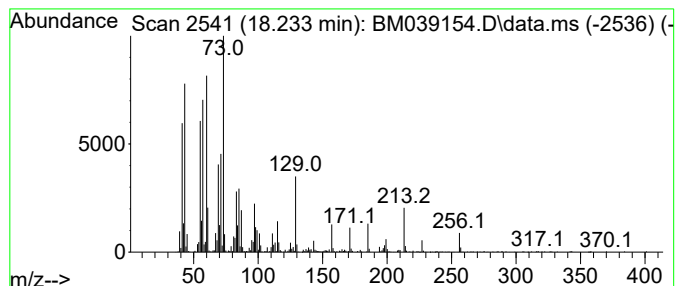
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	7.56 ng	1107680	Phenanthrene-d10	17.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	87



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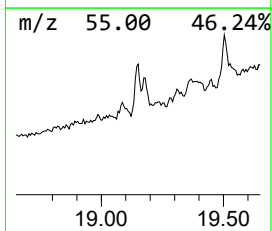
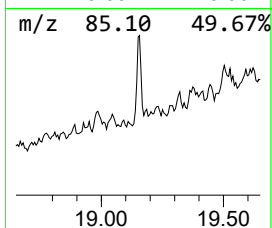
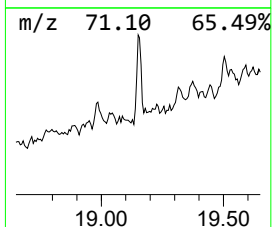
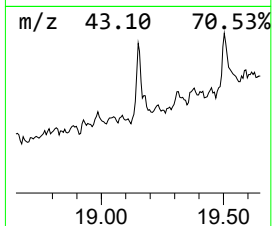
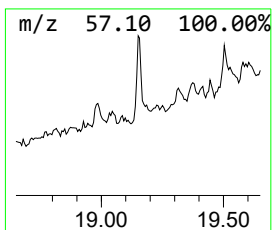
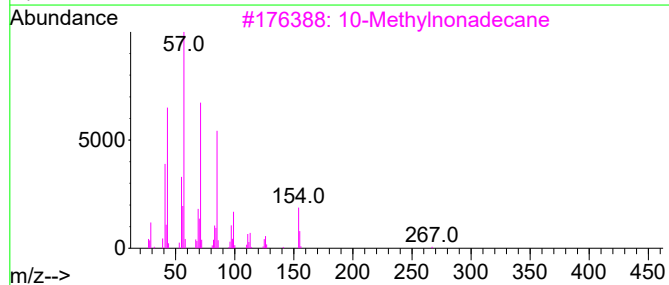
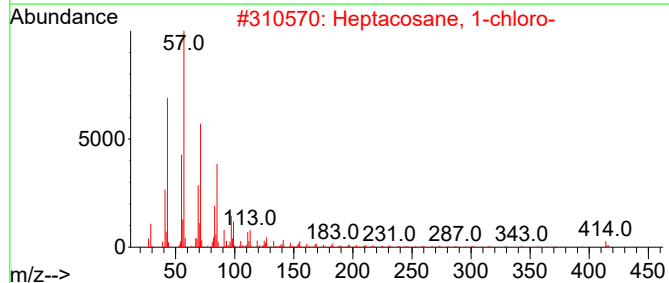
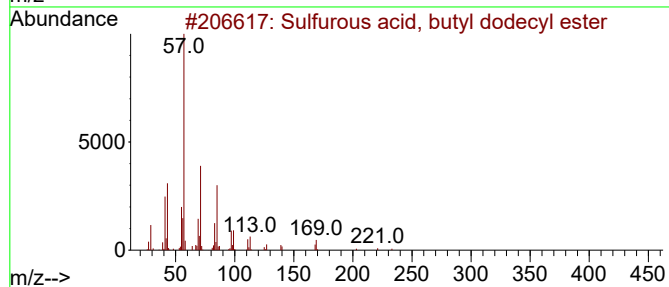
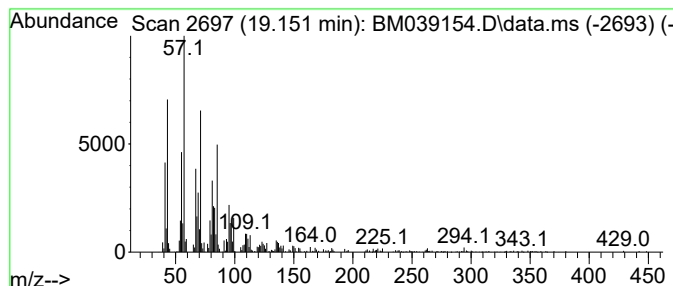
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Peak Number 4 Sulfurous acid, butyl dodec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.151	3.13 ng	458640	Phenanthrene-d10	17.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	53
2			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	53
3			10-Methylnonadecane	282	C20H42	056862-62-5	49
4			Pentacosane	352	C25H52	000629-99-2	49
5			1-Bromodocosane	388	C22H45Br	006938-66-5	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.040	21.0	ng	1563670	1	7.951	1488400	20.0
Benzophenone	15.951	5.0	ng	646913	3	14.592	2604530	20.0
n-Hexadecanoic ...	18.233	7.6	ng	1107680	4	17.339	2929600	20.0
Sulfurous acid,...	19.151	3.1	ng	458640	4	17.339	2929600	20.0