

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112122\
 Data File : BG055729.D
 Acq On : 22 Nov 2022 00:33
 Operator : CG/JU
 Sample : N5664-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-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-BG111622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055729.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.292	335	341	348	rBV	72114	113476	5.54%	1.023%
2	5.774	416	423	433	rBV	519021	843528	41.19%	7.601%
3	7.389	689	698	713	rBV	570276	979710	47.84%	8.828%
4	8.241	837	843	851	rBV	128310	219043	10.70%	1.974%
5	9.417	1034	1043	1054	rBV	332090	589421	28.78%	5.311%
6	11.073	1317	1325	1333	rBV	203566	368119	17.98%	3.317%
7	13.494	1728	1737	1748	rBV	944365	1498668	73.18%	13.504%
8	14.863	1963	1970	1978	rBV	354626	562829	27.48%	5.072%
9	16.209	2193	2199	2205	rVB	109017	157989	7.71%	1.424%
10	16.350	2216	2223	2236	rBV	759448	1175699	57.41%	10.594%
11	17.607	2430	2437	2442	rBV	437731	660741	32.27%	5.954%
12	17.771	2461	2465	2473	rVB3	17256	27582	1.35%	0.249%
13	18.465	2578	2583	2593	rBV	81038	141560	6.91%	1.276%
14	19.646	2779	2784	2790	rVB	51998	73813	3.60%	0.665%
15	19.728	2794	2798	2807	rVV4	25981	42305	2.07%	0.381%
16	20.004	2842	2845	2852	rVB	53916	78152	3.82%	0.704%
17	20.192	2871	2877	2883	rBV	1601445	2047851	100.00%	18.453%
18	21.902	3162	3168	3174	rBV	420650	687498	33.57%	6.195%
19	23.106	3369	3373	3380	rVB2	52601	97869	4.78%	0.882%
20	25.304	3739	3747	3760	rVB2	243324	731717	35.73%	6.593%

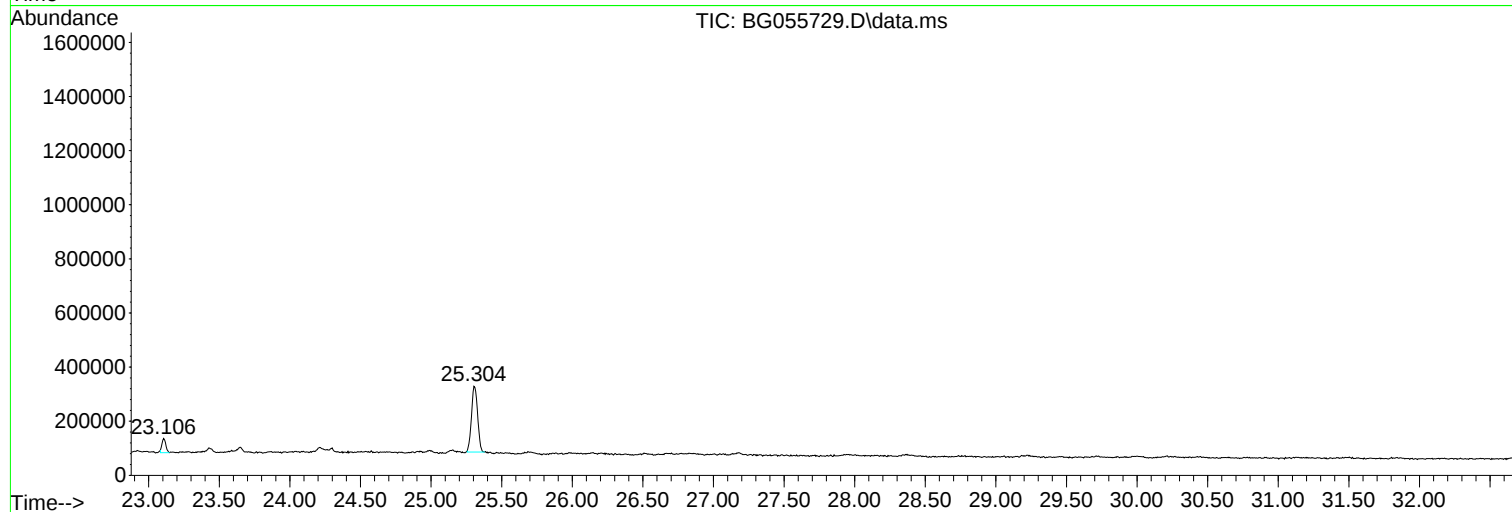
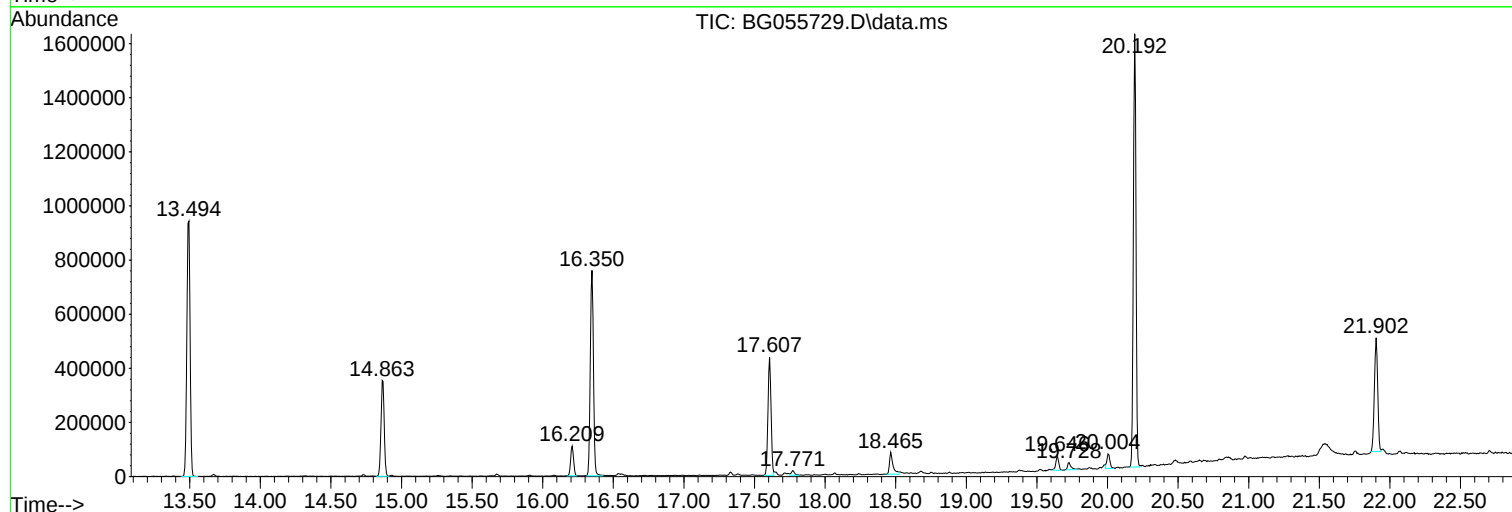
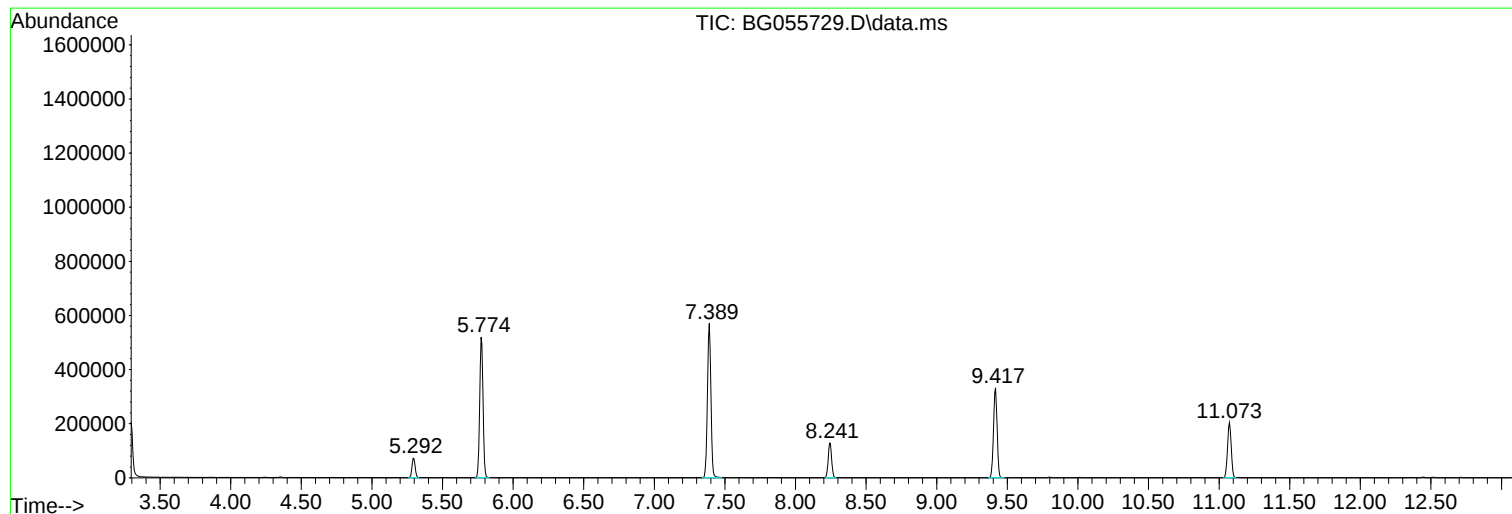
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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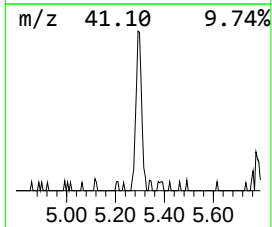
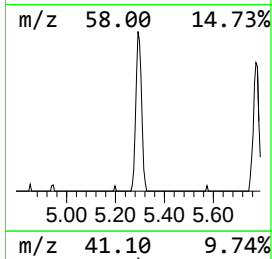
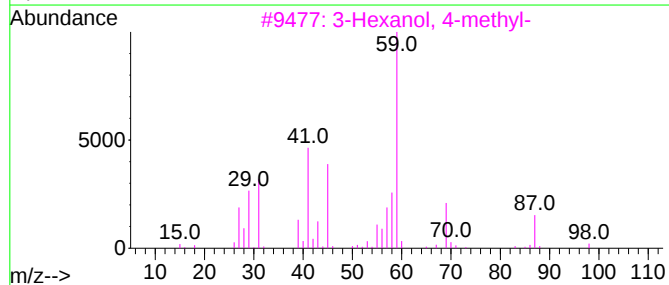
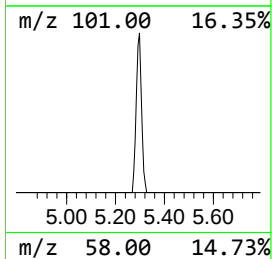
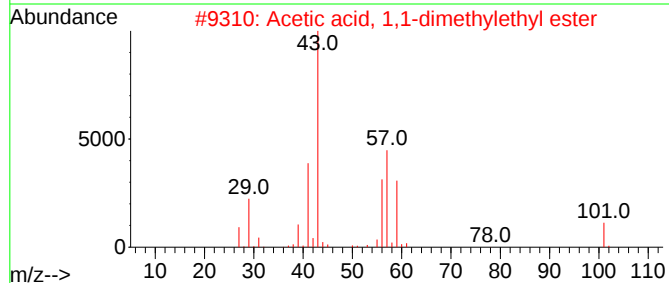
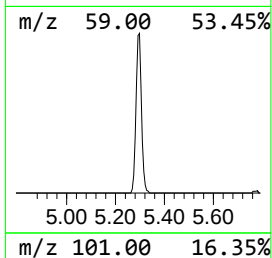
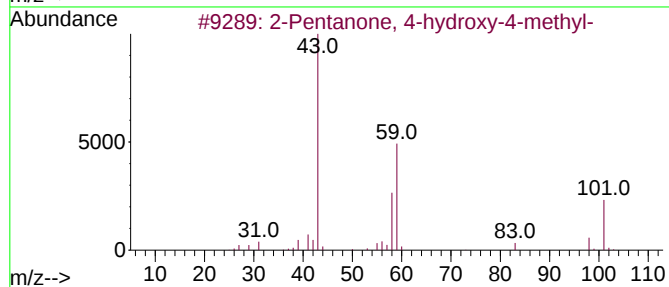
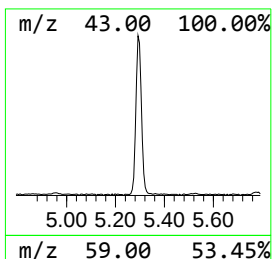
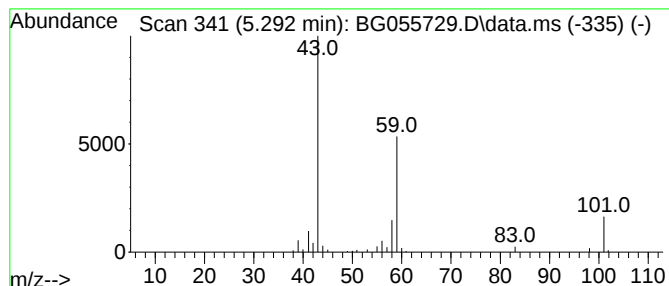
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.292	10.36 ng	113476	1,4-Dichlorobenzene-d4	8.241

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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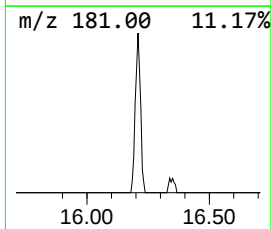
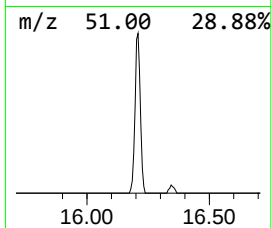
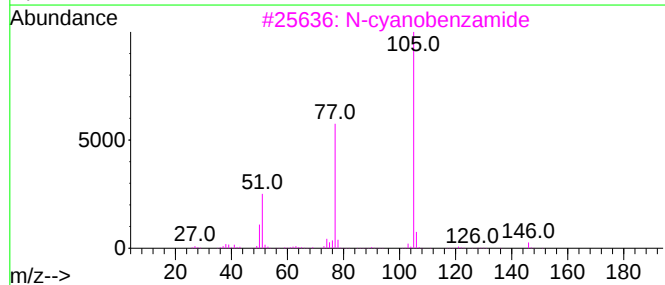
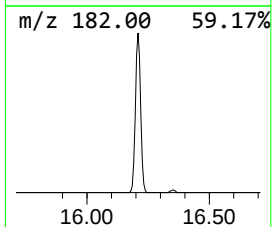
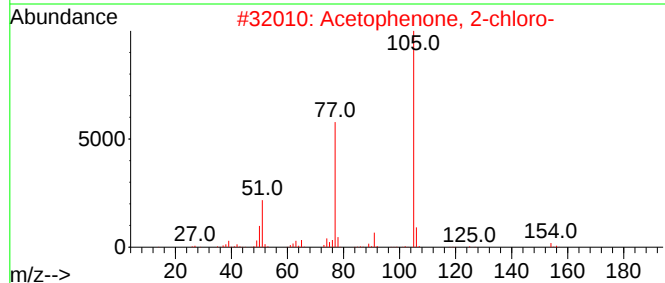
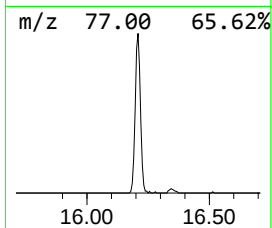
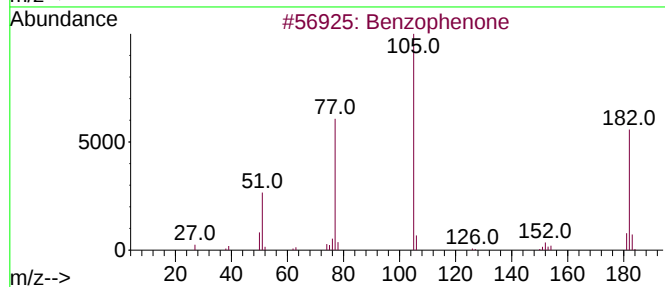
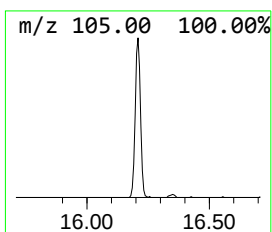
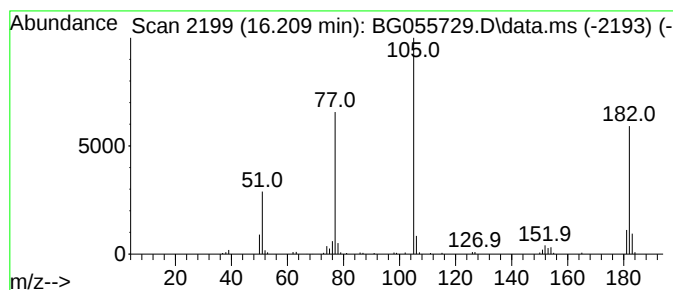
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.209	5.61 ng	157989	Acenaphthene-d10	14.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			N-cyanobenzamide	146	C8H6N2O	015150-25-1	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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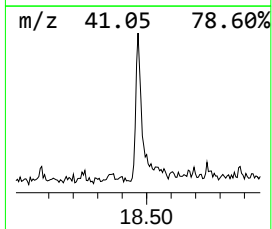
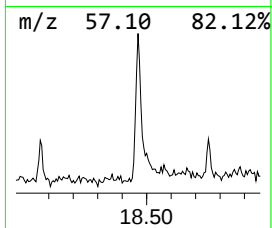
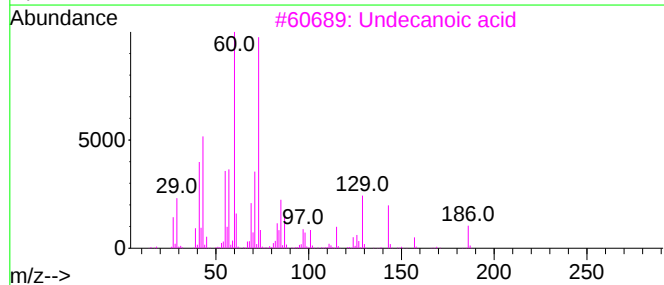
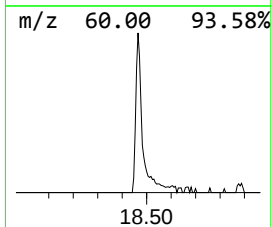
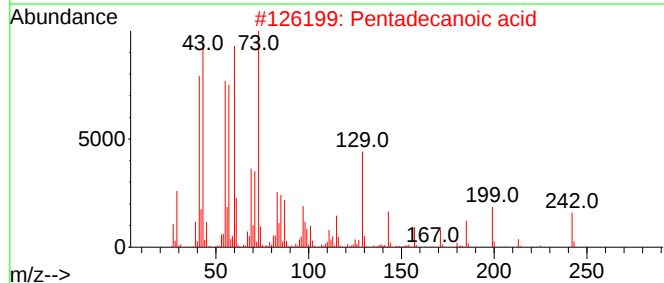
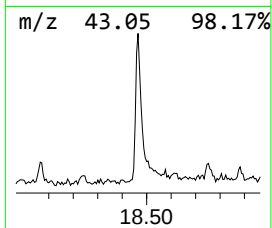
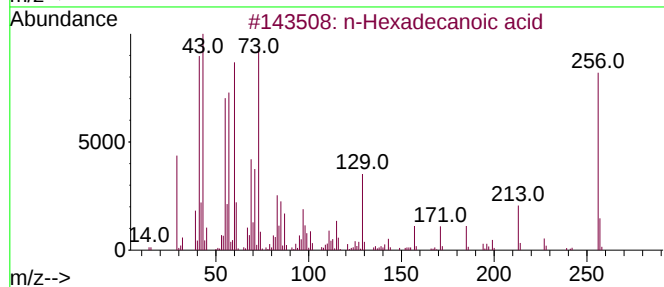
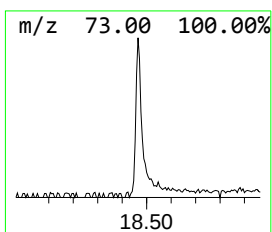
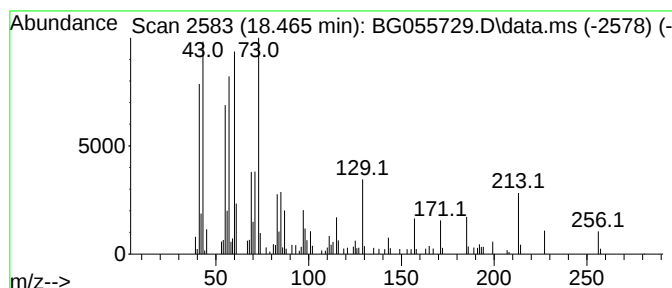
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.465	4.28 ng	141560	Phenanthrene-d10	17.607

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	83
3			Undecanoic acid	186	C11H22O2	000112-37-8	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



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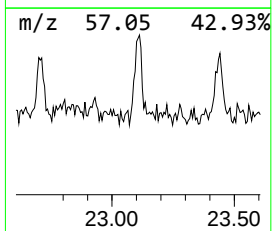
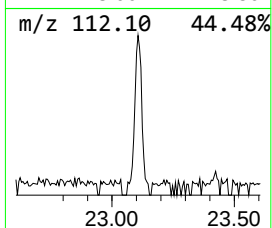
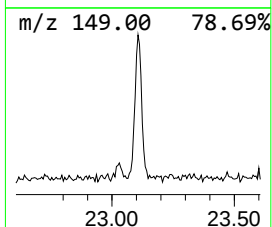
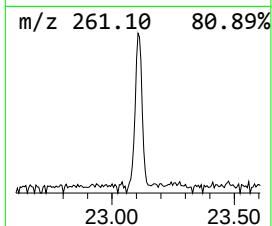
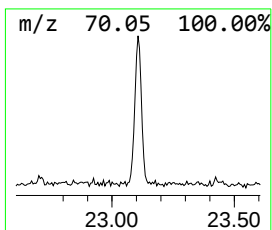
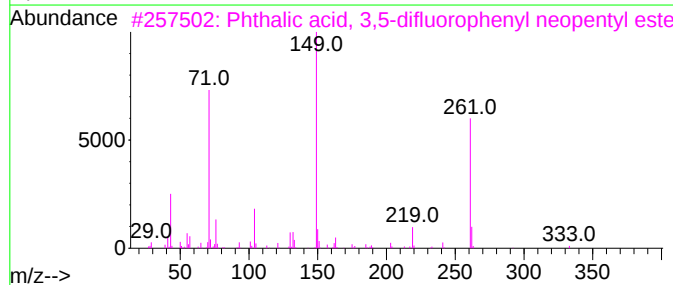
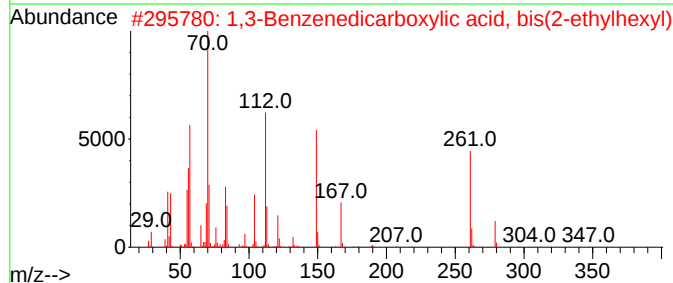
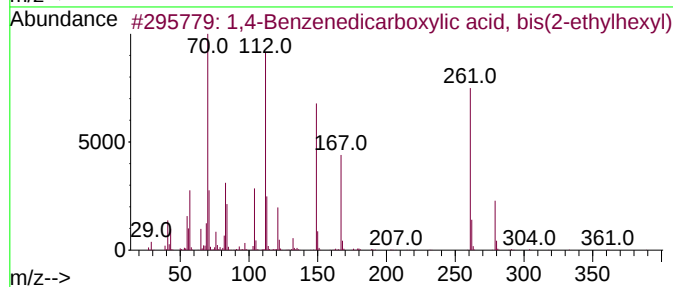
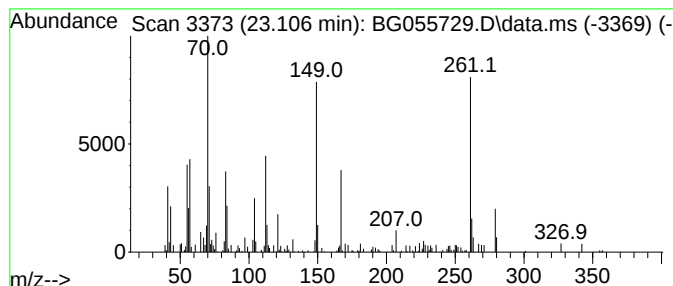
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Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
23.106	2.85 ng	97869	Chrysene-d12	21.902		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	80
2		1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64
3		Phthalic acid, 3,5-difluoropheny...	348	C19H18F2O4	1000315-54-1	35
4		Terephthalic acid, hept-3-yl oct...	376	C23H36O4	1000356-64-3	27
5		Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	14



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.292	10.4	ng	113476	1	8.241	219043	20.0
Benzophenone	16.209	5.6	ng	157989	3	14.863	562829	20.0
n-Hexadecanoic ...	18.465	4.3	ng	141560	4	17.607	660741	20.0
1,4-Benzenedica...	23.106	2.9	ng	97869	5	21.902	687498	20.0