

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042722\
 Data File : BG053352.D
 Acq On : 27 Apr 2022 18:06
 Operator : CG/JU
 Sample : N2482-12
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-23R

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-BG040822.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053352.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.667	382	388	400	rBV	353961	595071	17.10%	5.093%
2	7.264	653	660	672	rBV	273489	479918	13.79%	4.107%
3	7.869	757	763	771	rBV	27005	46954	1.35%	0.402%
4	8.104	796	803	808	rBV	91911	158213	4.55%	1.354%
5	8.157	808	812	820	rVB	64987	105776	3.04%	0.905%
6	9.268	993	1001	1009	rBV	411661	761217	21.87%	6.514%
7	10.912	1274	1281	1288	rBV	114013	212492	6.11%	1.819%
8	13.086	1646	1651	1660	rBV	22830	37291	1.07%	0.319%
9	13.350	1686	1696	1708	rBV	1104282	1792855	51.51%	15.343%
10	13.568	1726	1733	1750	rVB	374862	573867	16.49%	4.911%
11	14.725	1924	1930	1939	rVB	205018	325900	9.36%	2.789%
12	16.064	2152	2158	2162	rBV2	29349	40063	1.15%	0.343%
13	16.217	2177	2184	2195	rBV	985859	1588578	45.64%	13.595%
14	17.474	2391	2398	2411	rVB	296659	443966	12.76%	3.799%
15	20.076	2835	2841	2853	rVB	2644052	3480328	100.00%	29.785%
16	21.757	3120	3127	3137	rBV	313379	529042	15.20%	4.528%
17	25.052	3678	3688	3701	rVB2	176086	513459	14.75%	4.394%

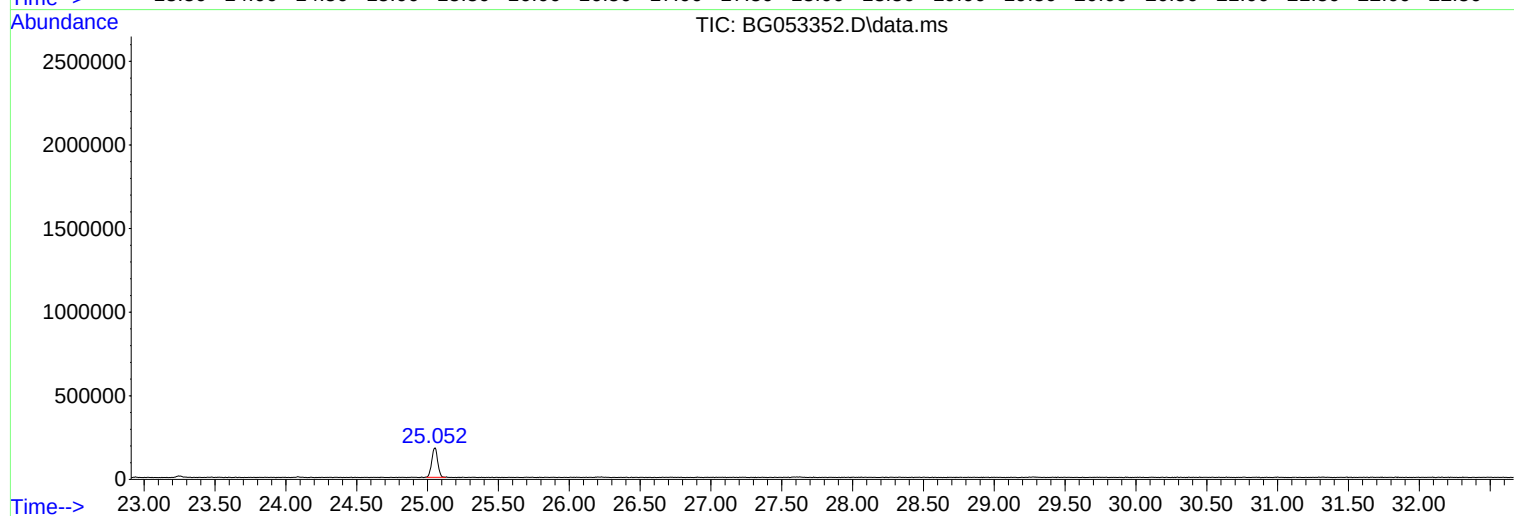
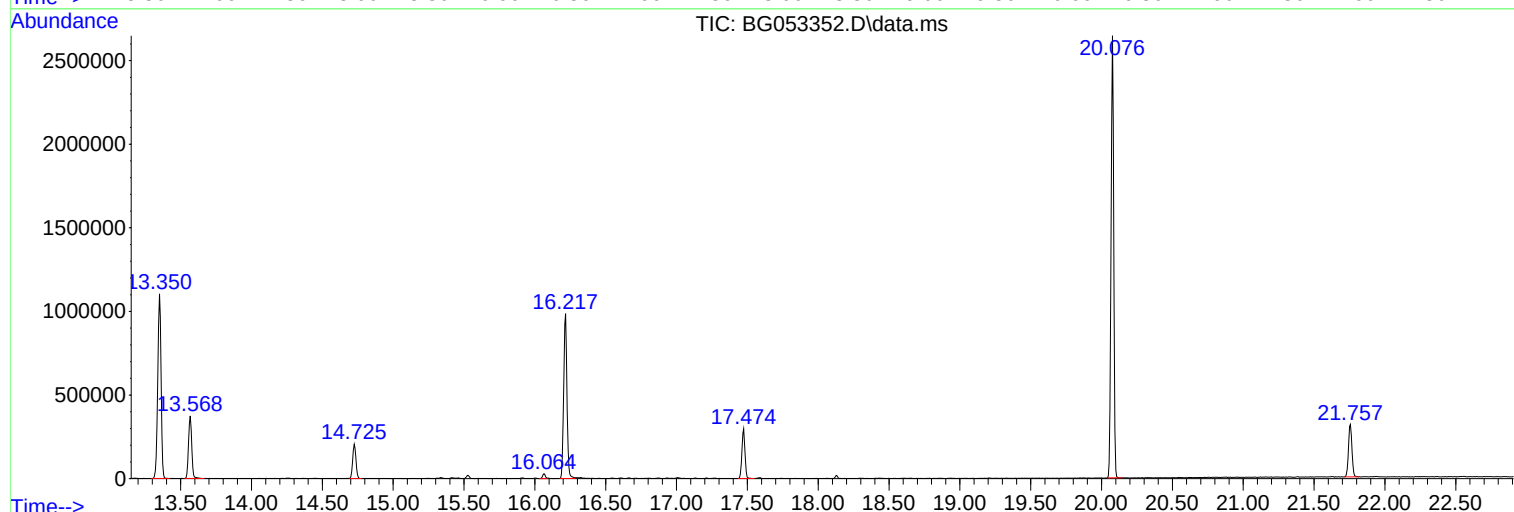
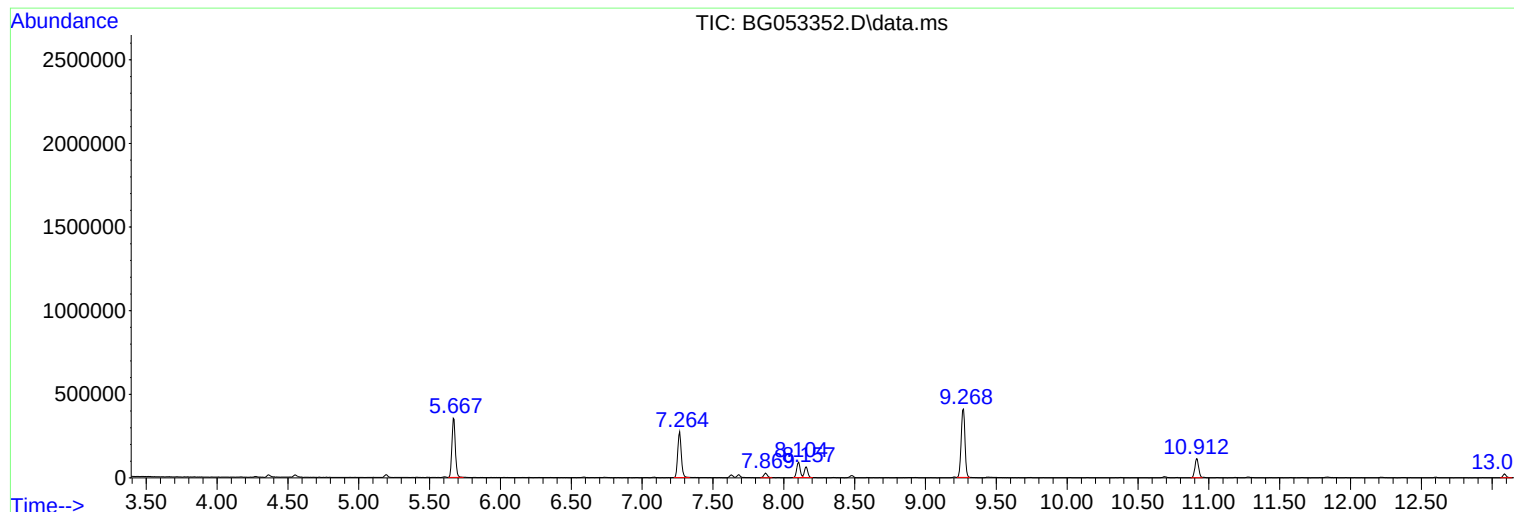
Sum of corrected areas: 11684990

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.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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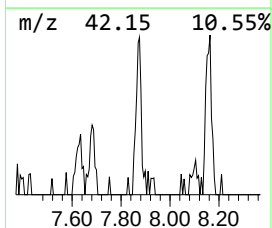
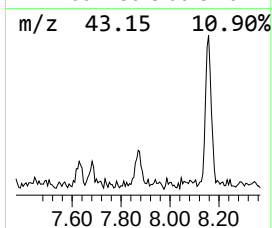
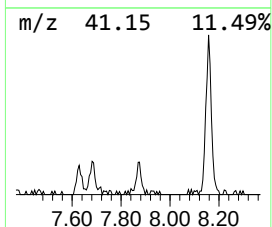
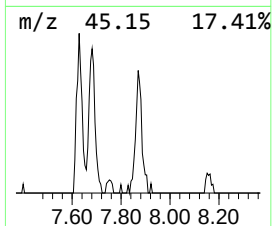
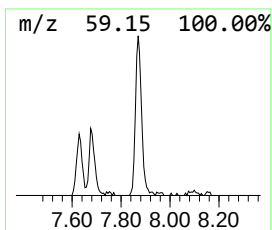
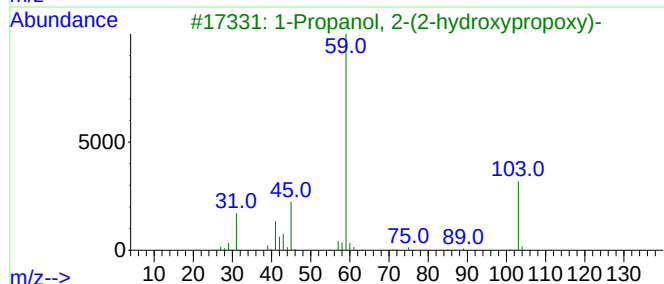
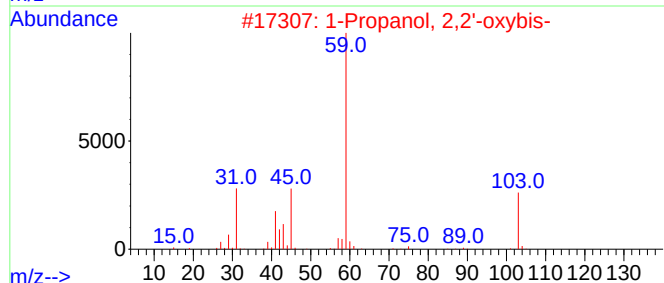
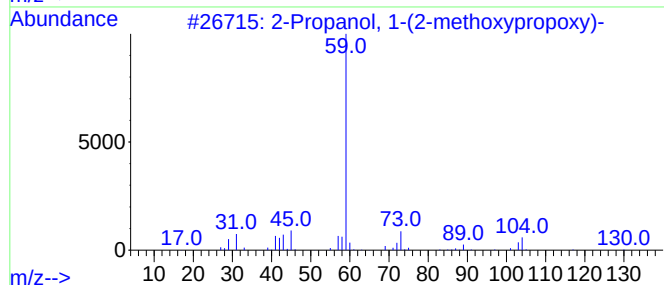
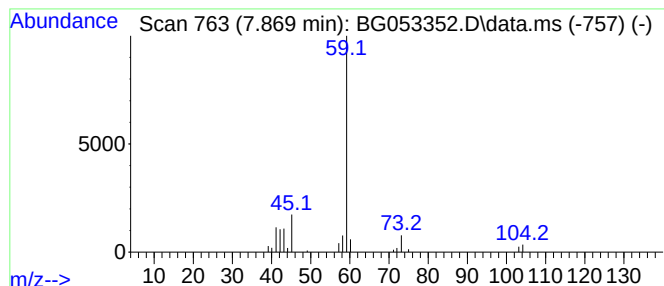
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG040822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.869	5.94 ng	46954	1,4-Dichlorobenzene-d4	8.104

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	74	
2	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	72	
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72	
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	72	
5	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	72	



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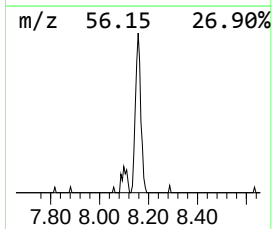
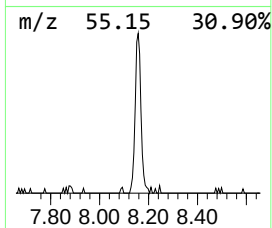
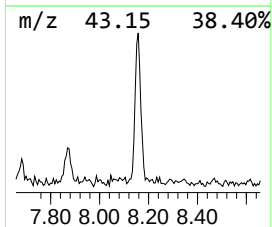
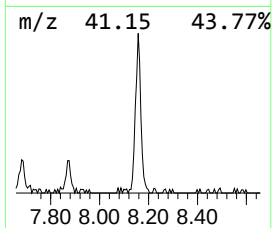
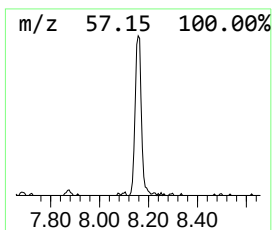
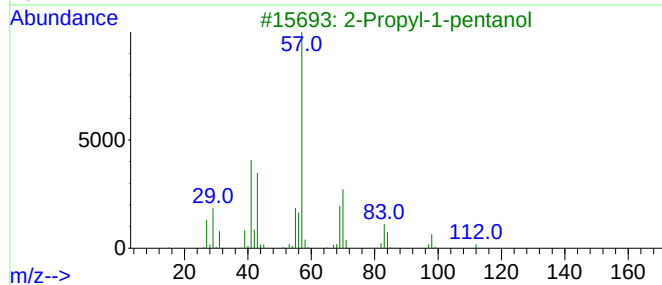
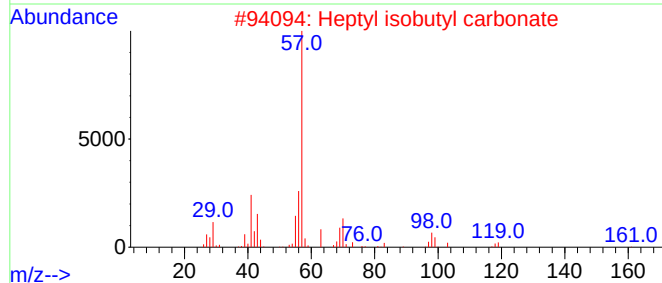
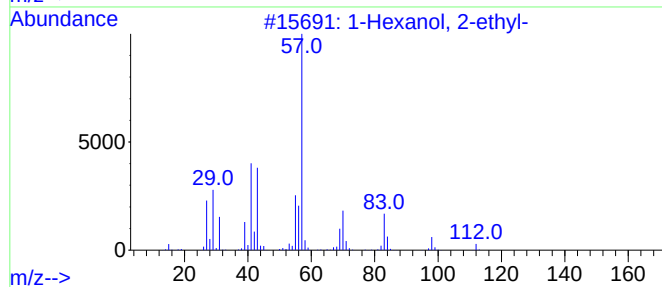
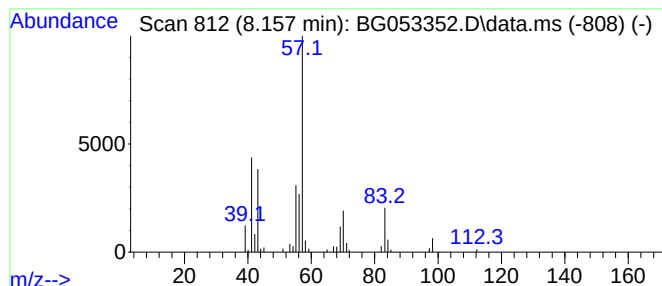
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.157	13.37 ng	105776	1,4-Dichlorobenzene-d4	8.104

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	47
5		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45



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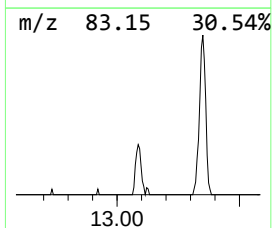
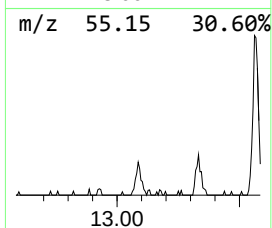
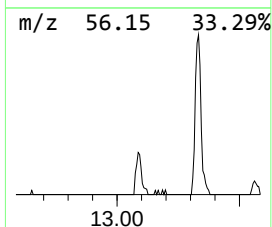
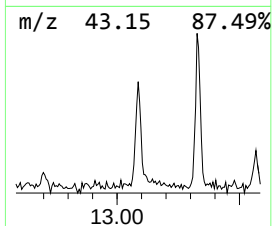
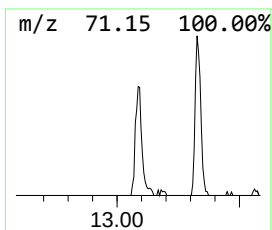
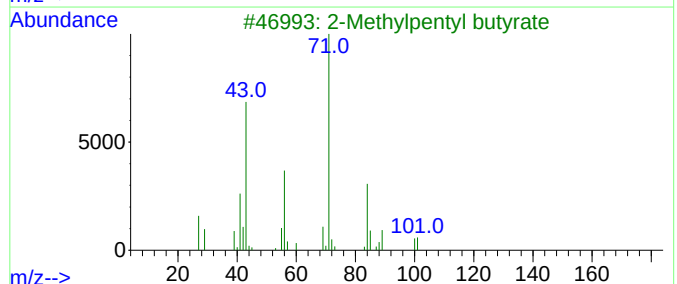
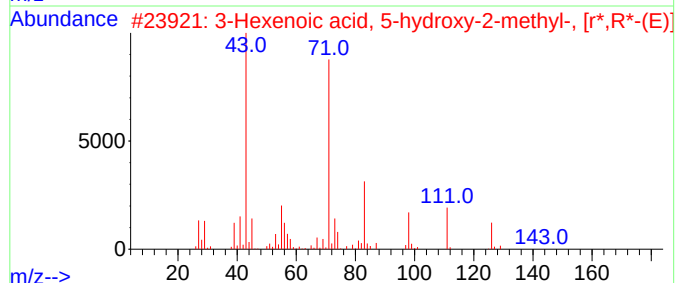
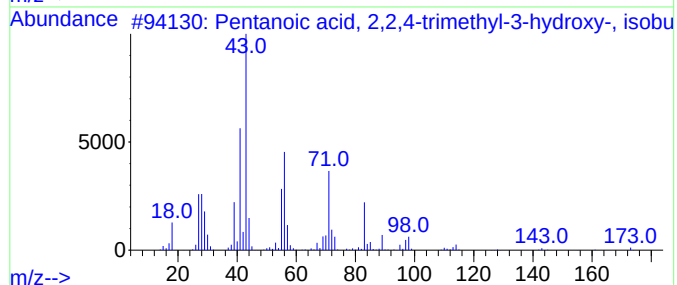
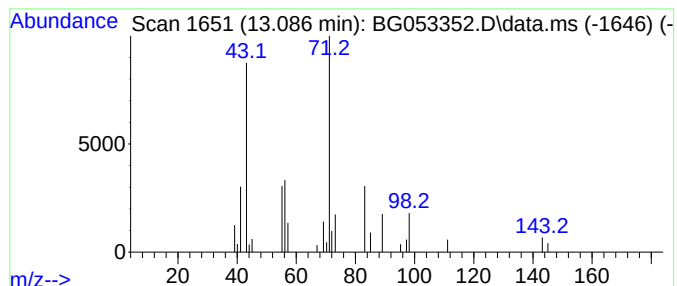
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Peak Number 3 Pentanoic acid, 2,2,4-trime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.086	2.29 ng	37291	Acenaphthene-d10	14.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 2,2,4-trimethyl-...	216	C12H24O3	244074-78-0	50
2			3-Hexenoic acid, 5-hydroxy-2-met...	144	C7H12O3	110678-36-9	42
3			2-Methylpentyl butyrate	172	C10H20O2	908106-67-2	42
4			Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	42
5			Diethylmalonic acid, monochlorid...	262	C12H19ClO4	1000370-65-0	38



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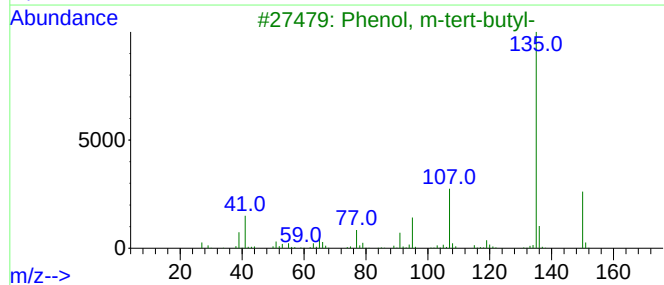
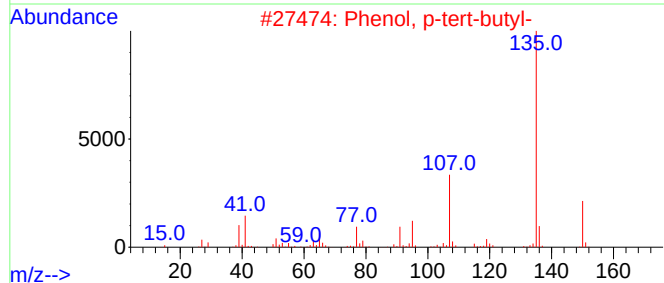
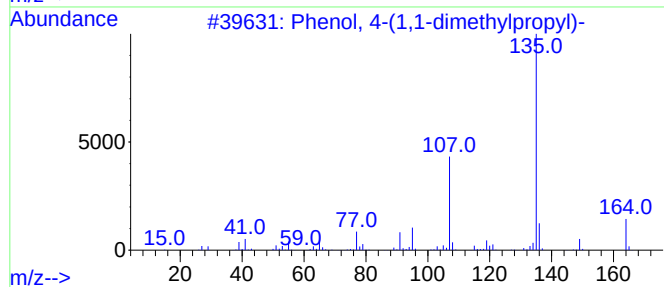
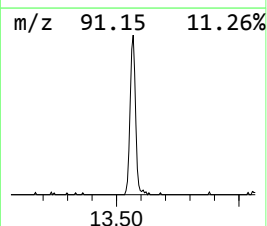
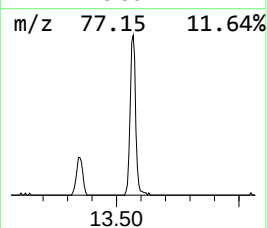
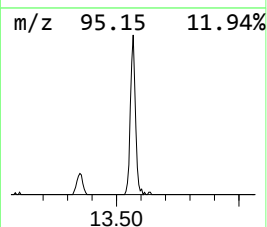
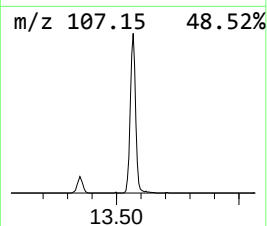
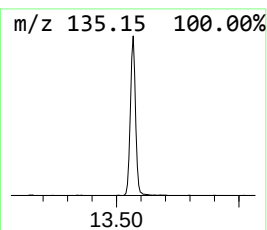
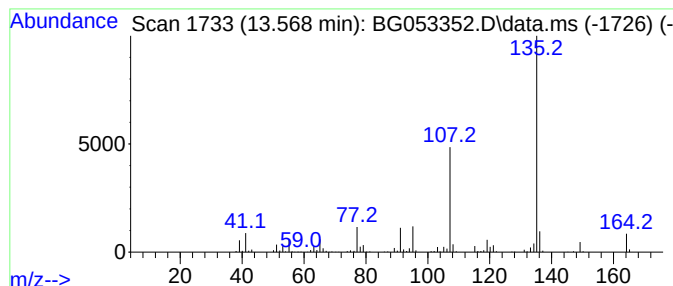
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Peak Number 4 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.568	35.22 ng	573867	Acenaphthene-d10	14.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	96
2			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3			Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	64
4			Phenol, 2-(1,1,3,3-tetramethylbu...	206	C14H22O	003884-95-5	64
5			Hexestrol	270	C18H22O2	000084-16-2	64



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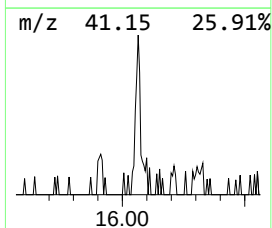
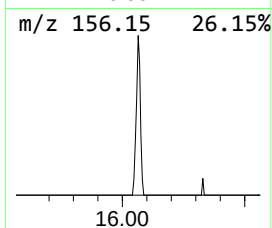
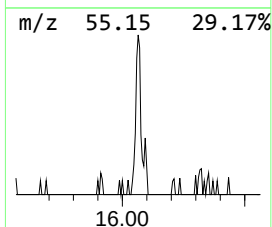
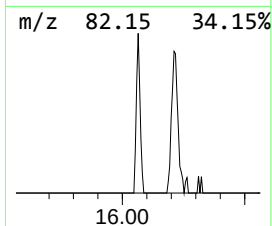
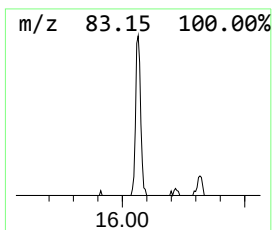
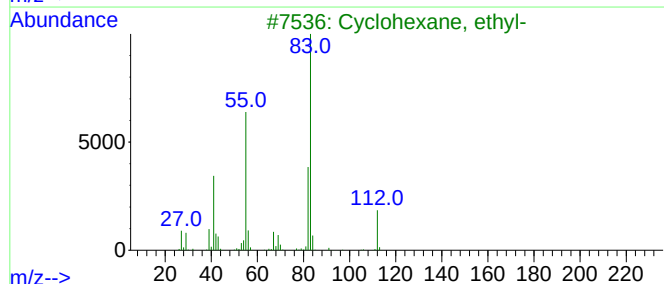
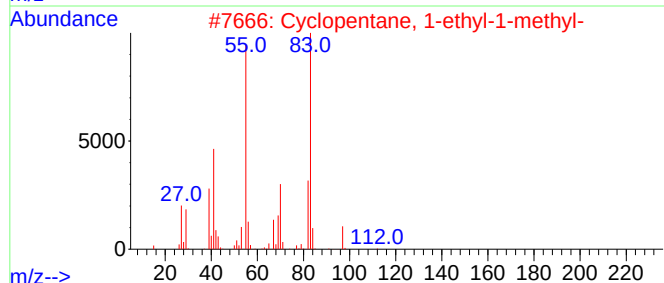
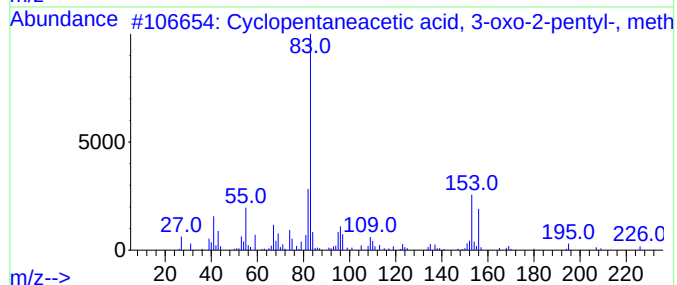
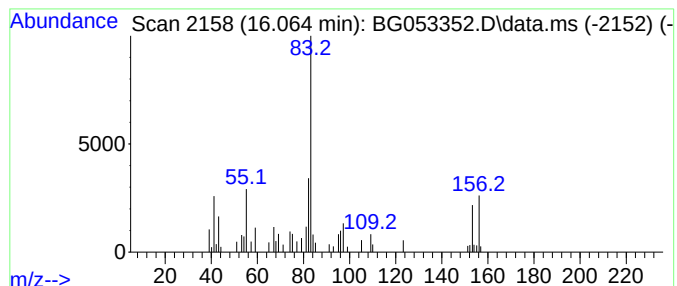
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Peak Number 5 Cyclopentaneacetic acid, 3-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.064	2.46 ng	40063	Acenaphthene-d10	14.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	86
2			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	47
3			Cyclohexane, ethyl-	112	C8H16	001678-91-7	37
4			Isocitronellol	156	C10H20O	018479-52-2	37
5			Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 1-(...	7.869	5.9	ng	46954	1	8.104	158213	20.0
1-Hexanol, 2-et...	8.157	13.4	ng	105776	1	8.104	158213	20.0
Pentanoic acid,...	13.086	2.3	ng	37291	3	14.725	325900	20.0
Phenol, 4-(1,1-...	13.568	35.2	ng	573867	3	14.725	325900	20.0
Cyclopentaneace...	16.064	2.5	ng	40063	3	14.725	325900	20.0