

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121423\
 Data File : BG060027.D
 Acq On : 15 Dec 2023 1:07
 Operator : MA/JU
 Sample : 05631-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-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-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060027.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.137	4	8	28	rVB	794016	1489822	14.73%	3.959%
2	5.059	330	335	343	rBV	137192	215199	2.13%	0.572%
3	5.523	407	414	425	rBV	959632	1588949	15.71%	4.222%
4	7.109	677	684	694	rVB	774124	1287246	12.72%	3.420%
5	7.955	820	828	835	rBV2	324359	537712	5.31%	1.429%
6	9.119	1013	1026	1033	rBV	1205553	2106417	20.82%	5.597%
7	9.230	1037	1045	1049	rBV3	71816	130225	1.29%	0.346%
8	10.758	1296	1305	1315	rBV	444907	755333	7.47%	2.007%
9	13.220	1716	1724	1733	rVB	3612100	5636103	55.71%	14.976%
10	14.383	1915	1922	1928	rBV	80844	139223	1.38%	0.370%
11	14.594	1949	1958	1967	rBV	785552	1273933	12.59%	3.385%
12	16.081	2204	2211	2218	rBV	4250916	6168758	60.97%	16.391%
13	17.338	2419	2425	2432	rBV	1199577	1789202	17.68%	4.754%
14	18.231	2573	2577	2582	rBV	265939	356591	3.52%	0.947%
15	19.506	2791	2794	2798	rBV4	100311	120220	1.19%	0.319%
16	19.965	2866	2872	2878	rBV	7883549	10117103	100.00%	26.882%
17	21.610	3146	3152	3158	rBV2	1194916	1893744	18.72%	5.032%
18	24.800	3685	3695	3709	rVB2	720852	2029158	20.06%	5.392%

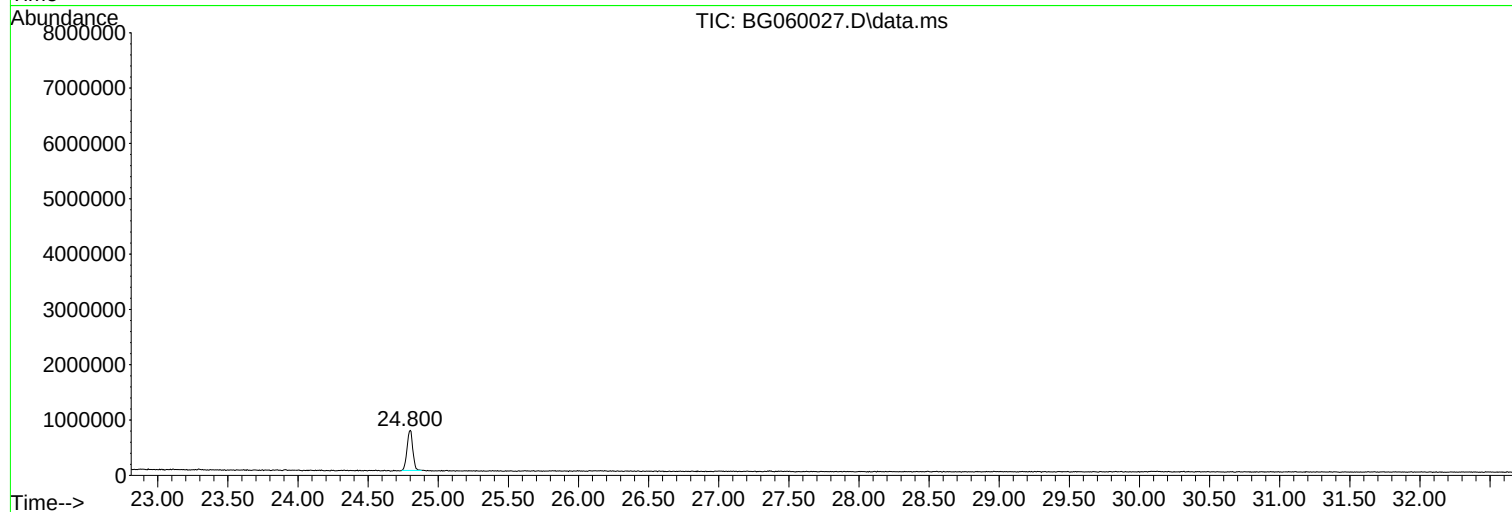
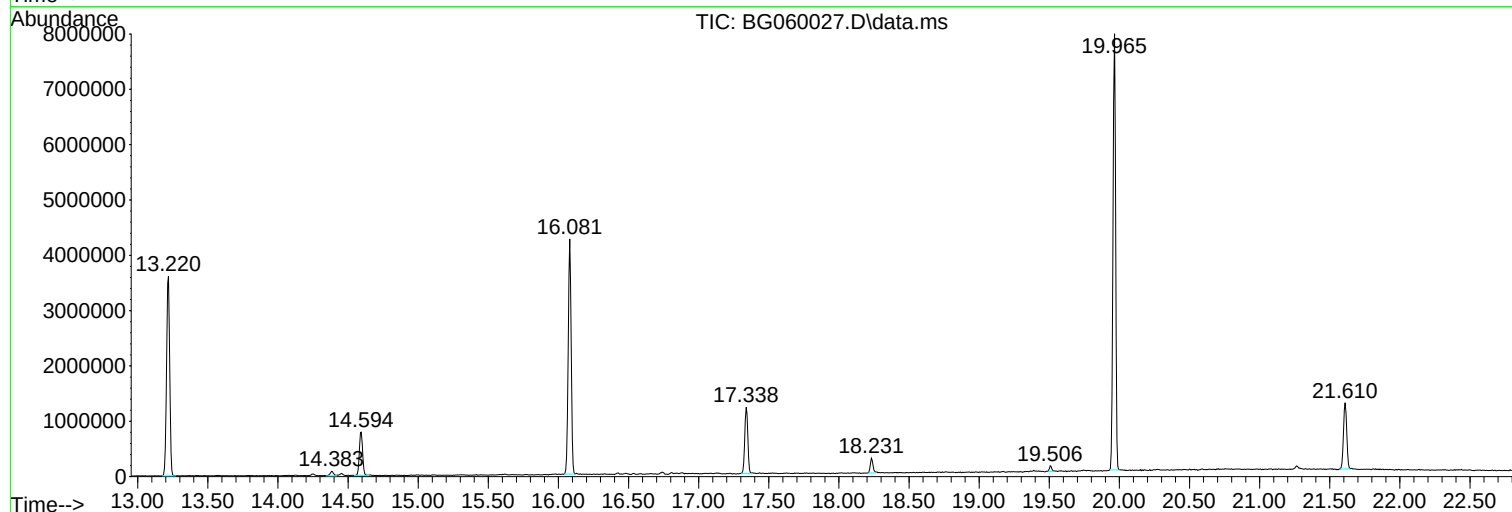
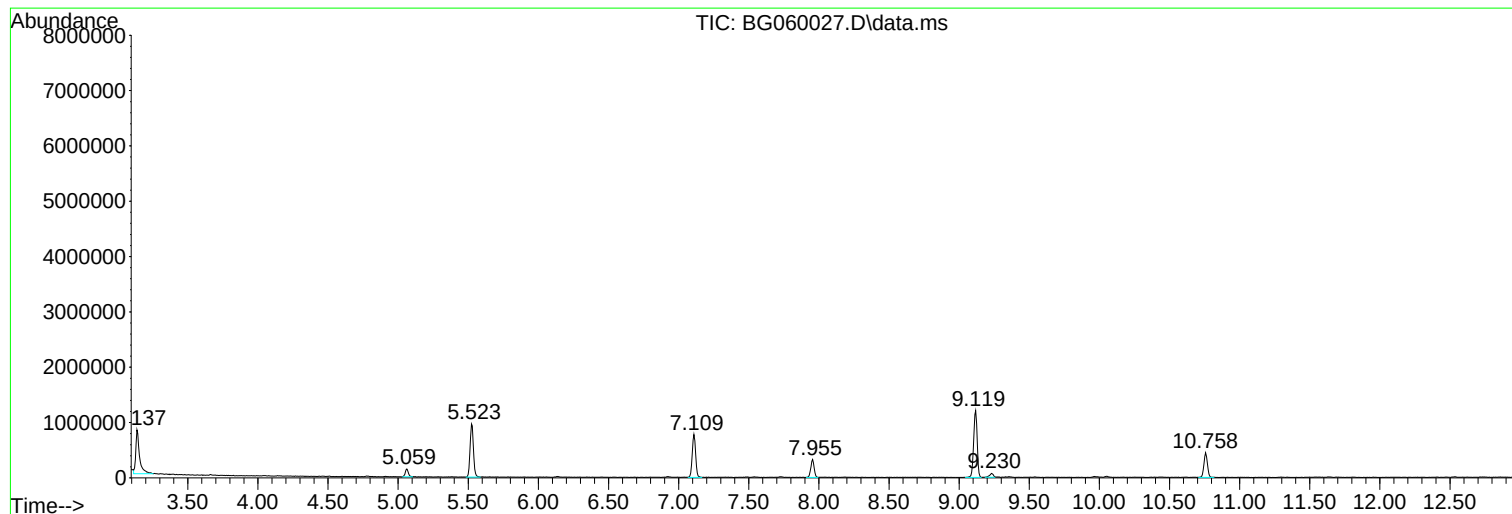
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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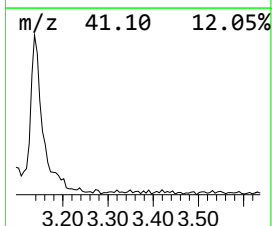
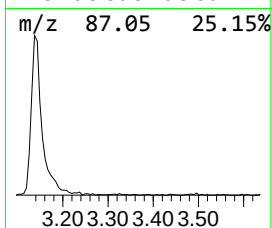
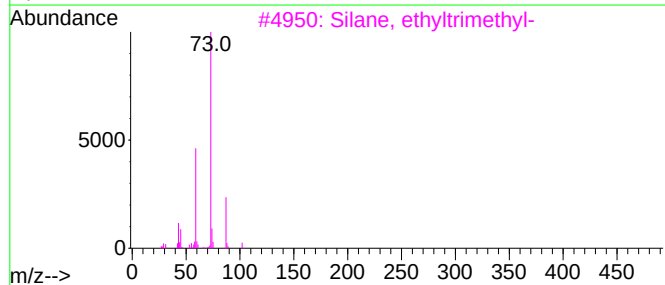
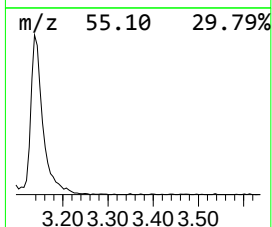
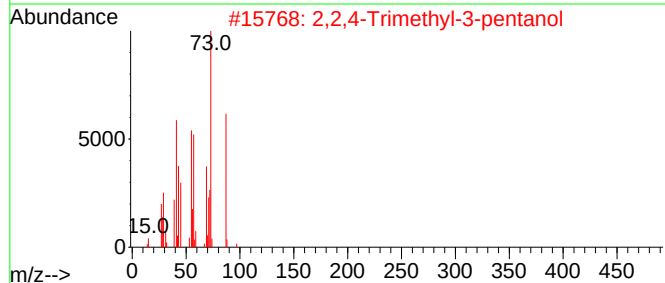
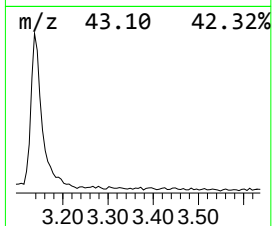
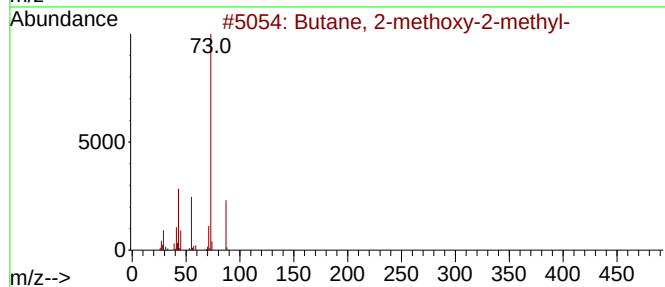
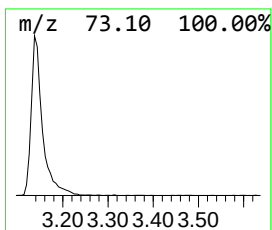
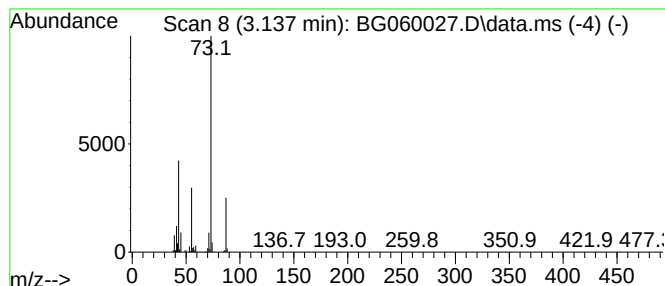
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.137	55.41 ng	1489820	1,4-Dichlorobenzene-d4	7.955

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	38
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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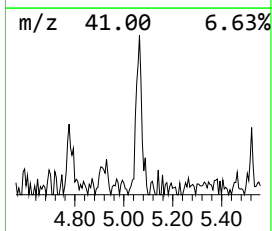
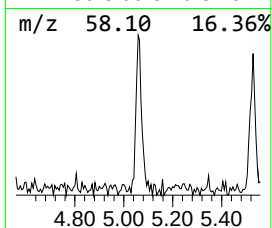
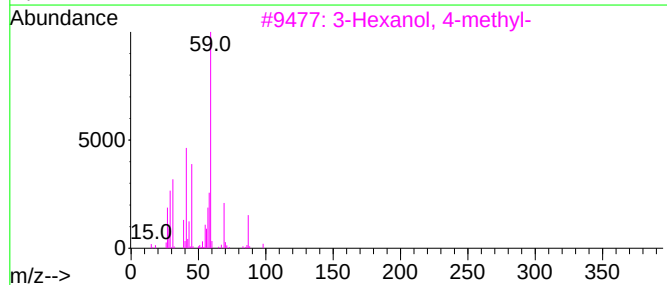
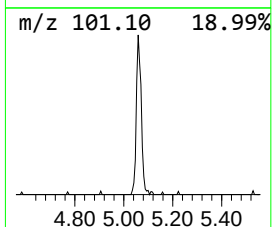
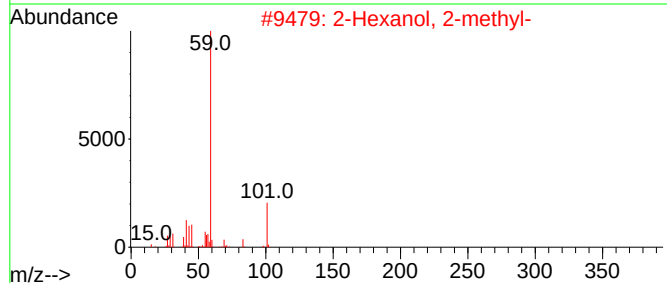
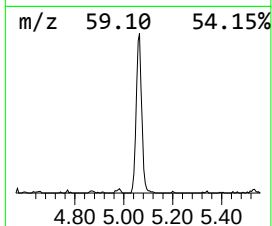
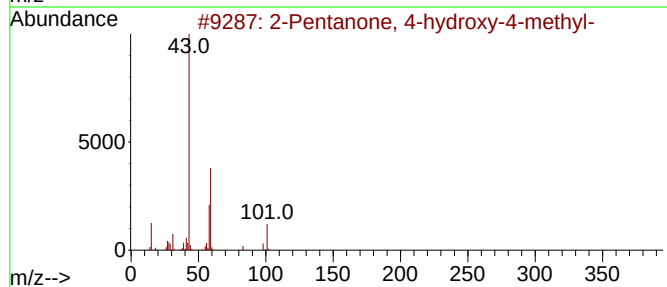
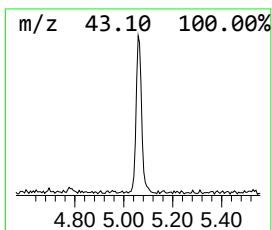
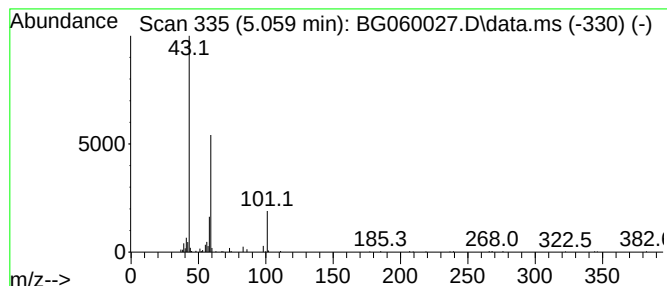
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.059	8.00 ng	215199	1,4-Dichlorobenzene-d4	7.955

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	23
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5		1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	17



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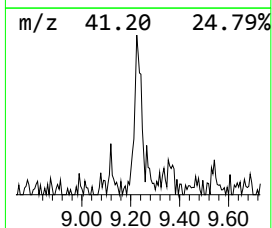
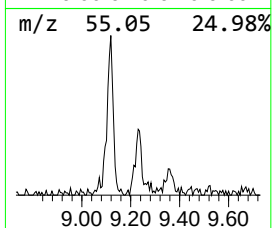
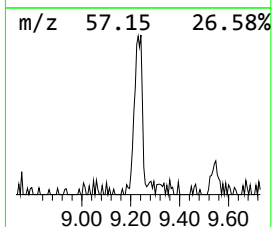
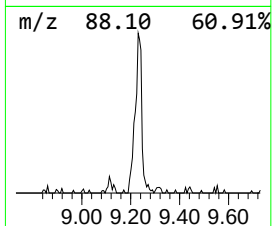
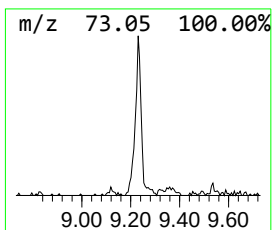
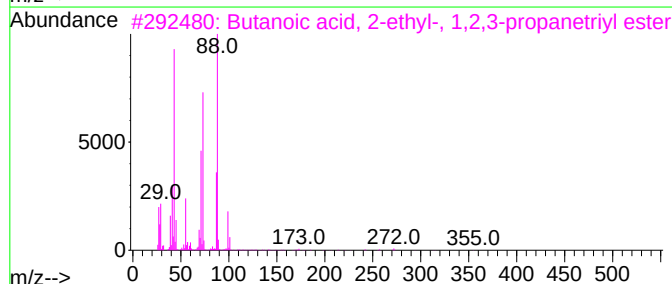
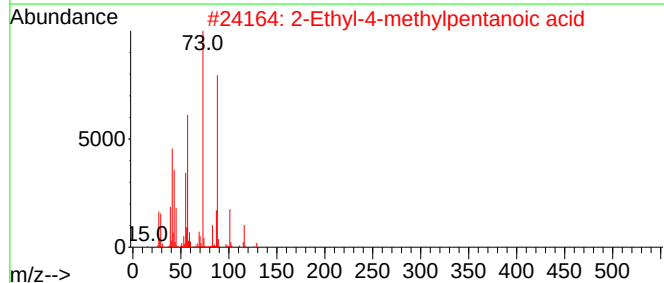
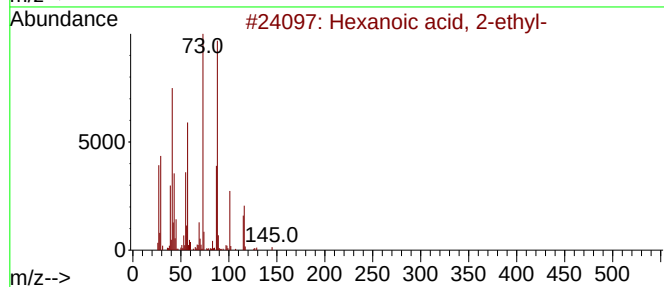
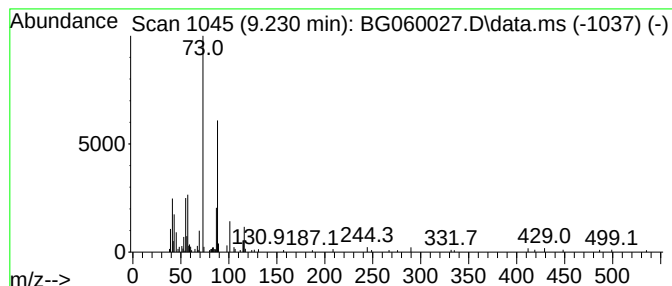
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Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.230	4.84 ng	130225	1,4-Dichlorobenzene-d4	7.955

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	53
2			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	47
3			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
4			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	42
5			Sulfide, allyl methyl	88	C4H8S	010152-76-8	38



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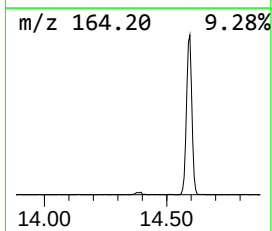
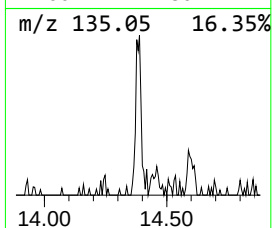
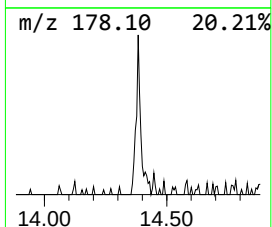
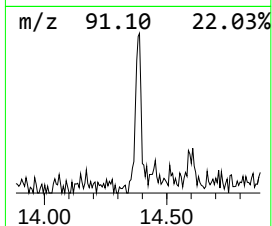
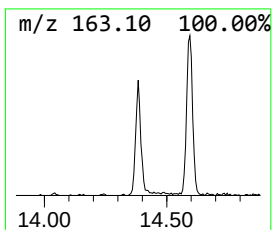
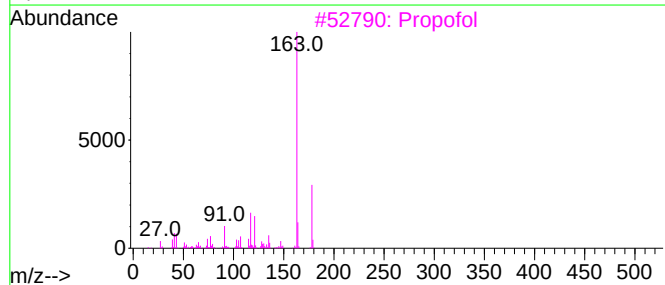
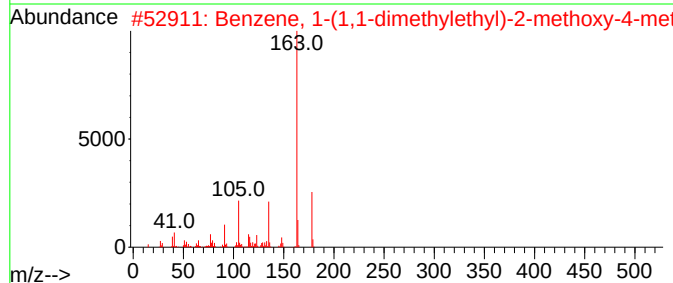
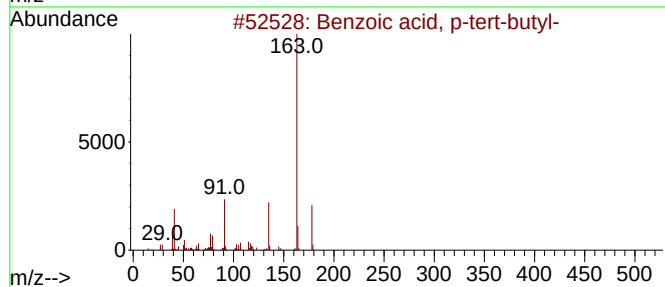
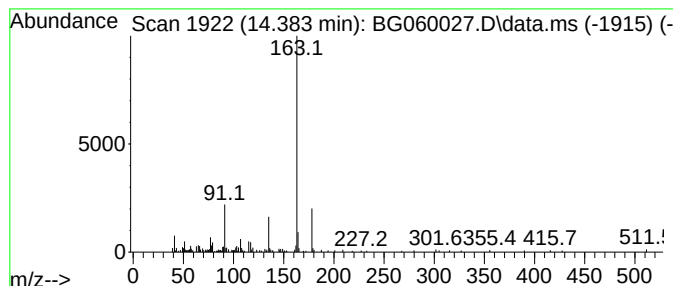
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Peak Number 4 Benzoic acid, p-tert-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.383	2.19 ng	139223	Acenaphthene-d10	14.594

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	90
2			Benzene, 1-(1,1-dimethylethyl)-2...	178	C12H18O	000088-40-4	80
3			Propofol	178	C12H18O	002078-54-8	80
4			4-tert-Butyl-2,6-dimethylphenol	178	C12H18O	000879-97-0	80
5			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	80



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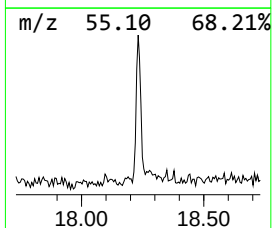
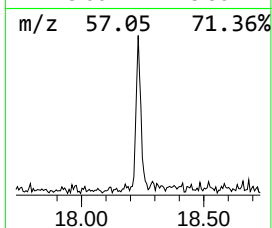
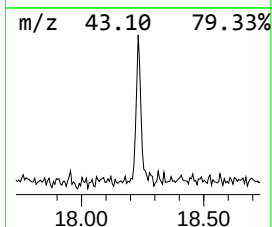
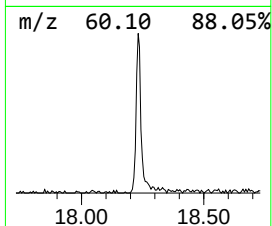
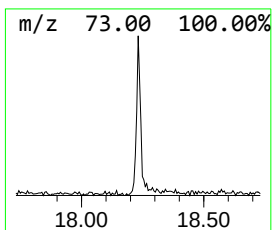
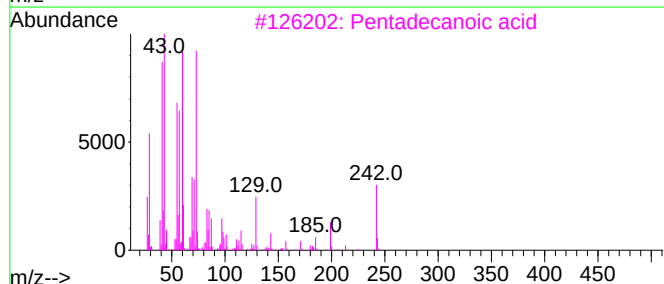
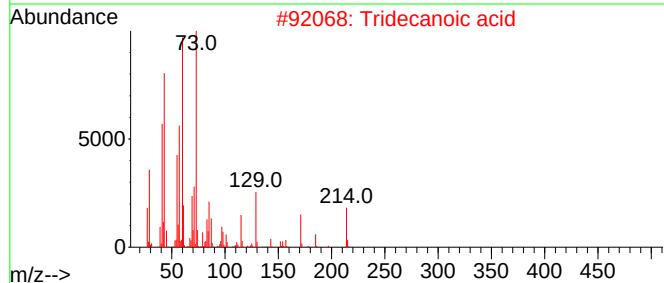
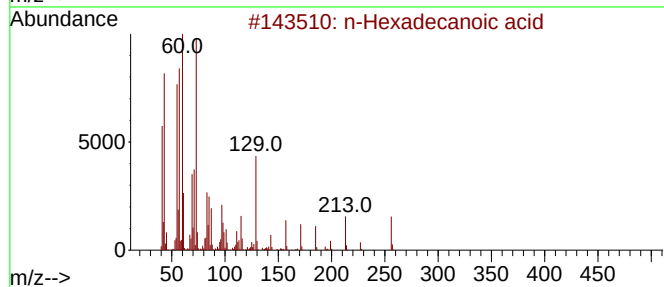
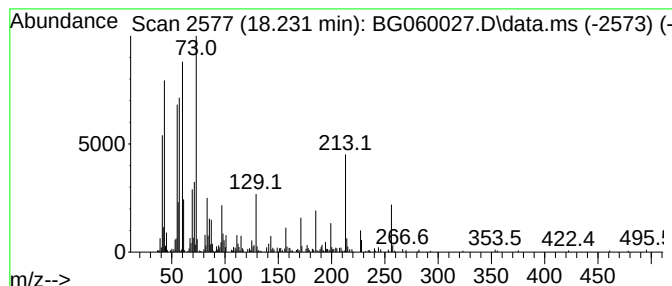
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.231	3.99 ng	356591	Phenanthrene-d10	17.338

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	49
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4			Dodecanoic acid	200	C12H24O2	000143-07-7	46
5			Nonanoic acid	158	C9H18O2	000112-05-0	45



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.137	55.4	ng	1489820	1	7.955	537712	20.0
2-Pentanone, 4-...	5.059	8.0	ng	215199	1	7.955	537712	20.0
Hexanoic acid, ...	9.230	4.8	ng	130225	1	7.955	537712	20.0
Benzoic acid, p...	14.383	2.2	ng	139223	3	14.594	1273930	20.0
n-Hexadecanoic ...	18.231	4.0	ng	356591	4	17.338	1789200	20.0