

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061721\
 Data File : BG049013.D
 Acq On : 17 Jun 2021 14:21
 Operator : CG/JU
 Sample : M2735-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 124035

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-BG061121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049013.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.155	14	20	30	rBV	82461	170536	8.97%	1.728%
2	3.238	30	34	39	rVB	20669	31568	1.66%	0.320%
3	5.188	361	366	376	rBV2	12076	23477	1.24%	0.238%
4	5.664	440	447	456	rVB	493041	817693	43.02%	8.284%
5	7.262	711	719	727	rBV	510945	885288	46.58%	8.968%
6	8.108	857	863	870	rVB	129553	220669	11.61%	2.235%
7	9.278	1053	1062	1072	rBV	309741	559920	29.46%	5.672%
8	10.694	1296	1303	1312	rBV	100795	179314	9.43%	1.817%
9	10.934	1336	1344	1350	rBV	158676	283655	14.92%	2.874%
10	13.379	1751	1760	1767	rBV	710721	1124127	59.14%	11.388%
11	14.754	1988	1994	2001	rVB	260272	413252	21.74%	4.186%
12	16.240	2240	2247	2254	rBV	706232	1089769	57.34%	11.040%
13	17.503	2455	2462	2468	rBV	355064	554028	29.15%	5.613%
14	18.379	2606	2611	2621	rBV2	79391	121656	6.40%	1.232%
15	19.654	2824	2828	2833	rBV3	30268	43829	2.31%	0.444%
16	20.106	2900	2905	2912	rBV	1462120	1900653	100.00%	19.254%
17	21.422	3124	3129	3138	rBV	81405	137447	7.23%	1.392%
18	21.792	3184	3192	3198	rBV	364491	622623	32.76%	6.307%
19	21.998	3222	3227	3233	rBV6	10271	22539	1.19%	0.228%
20	22.633	3330	3335	3342	rBV10	12506	28224	1.48%	0.286%
21	25.124	3749	3759	3771	rBV2	214944	618215	32.53%	6.263%
22	26.493	3986	3992	3995	rBV5	10505	22830	1.20%	0.231%

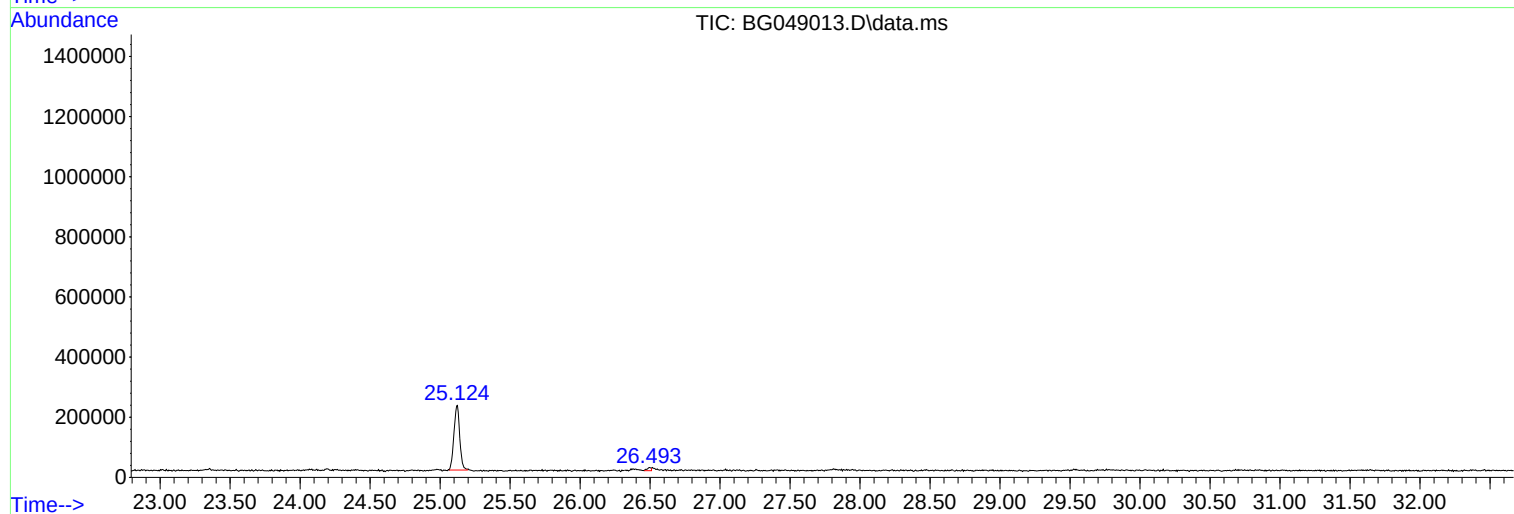
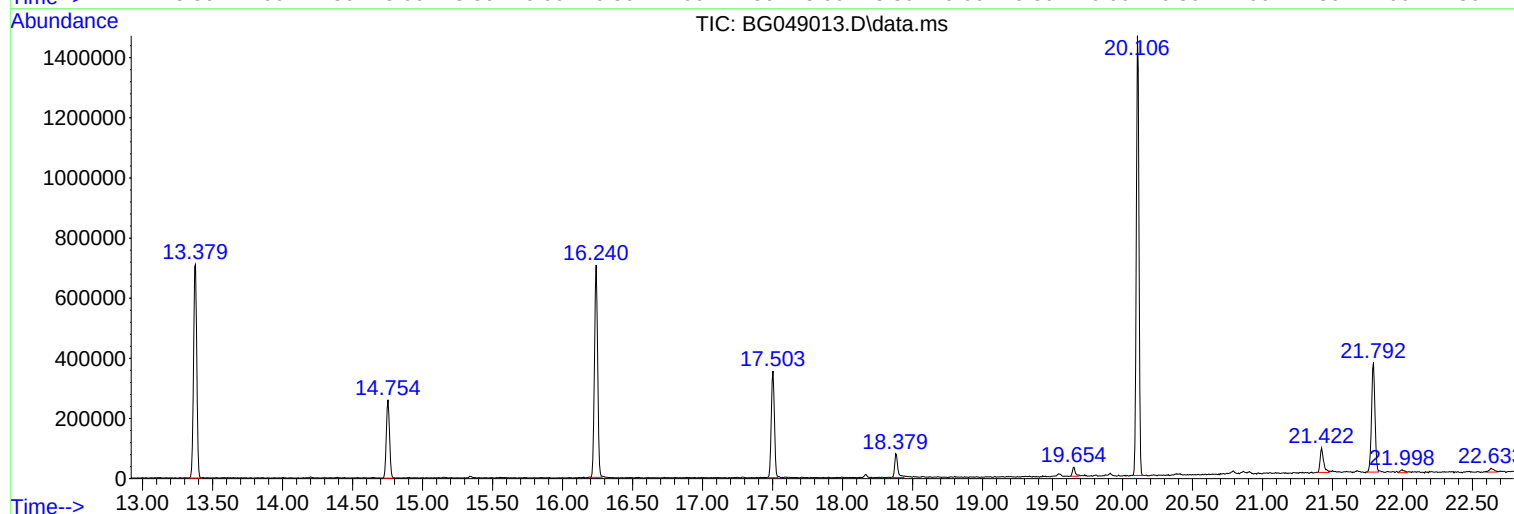
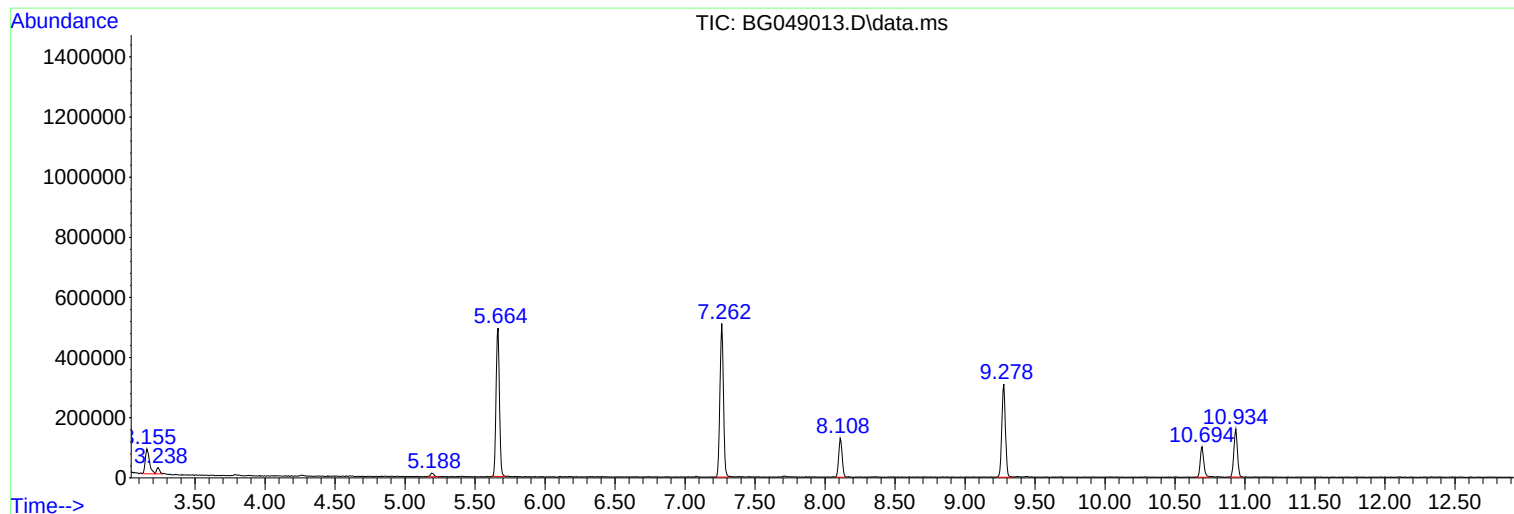
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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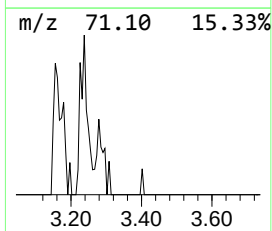
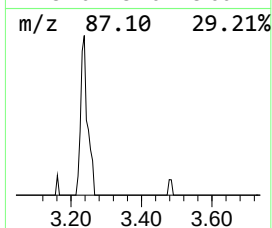
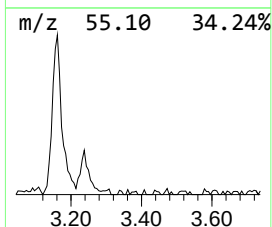
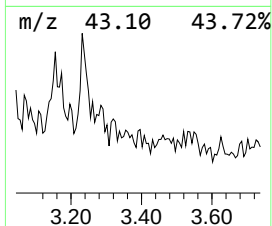
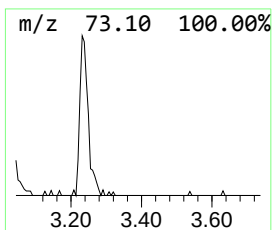
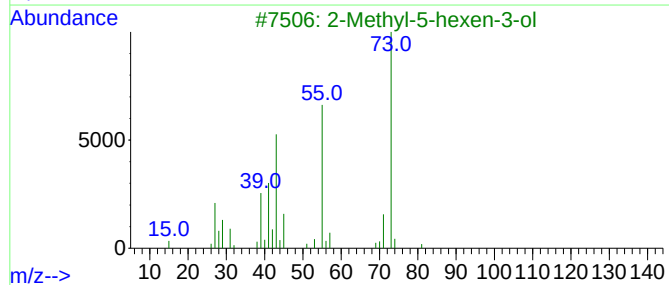
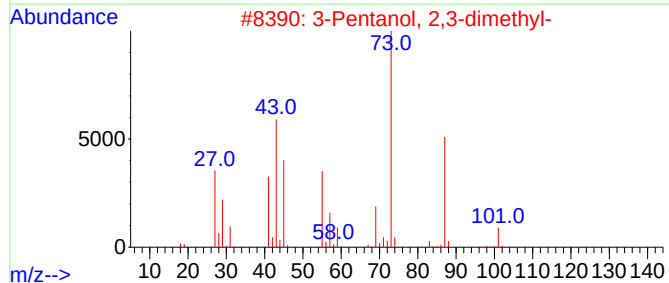
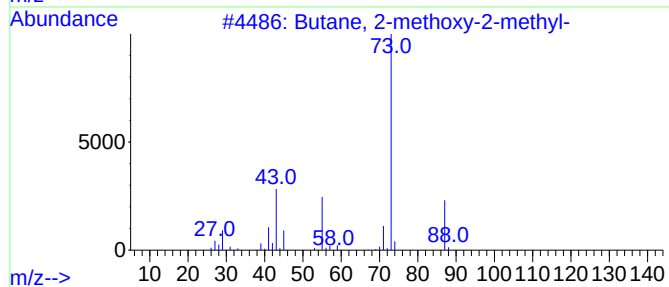
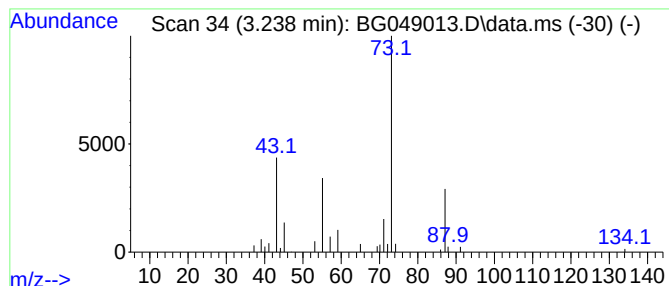
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.238	2.86 ng	31568	1,4-Dichlorobenzene-d4	8.114

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	50
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	33
5			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25



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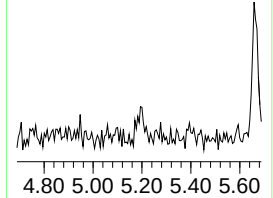
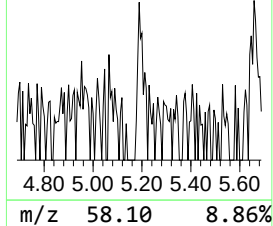
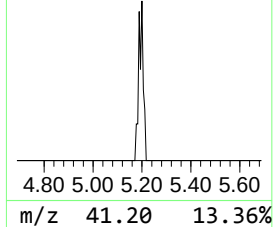
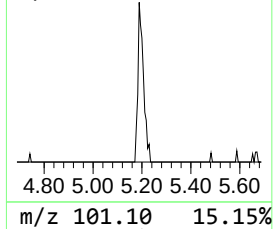
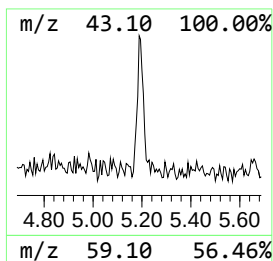
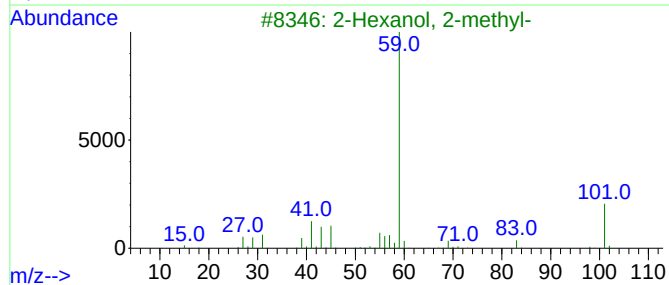
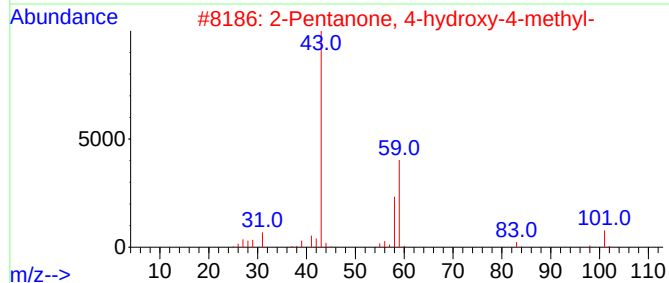
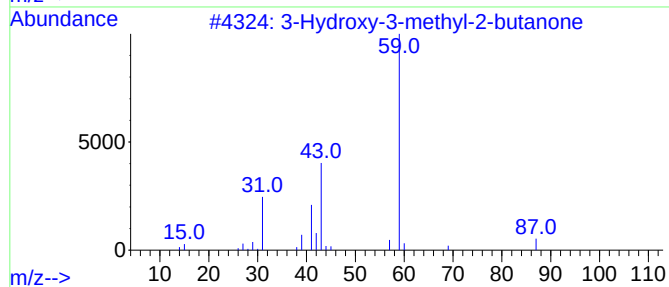
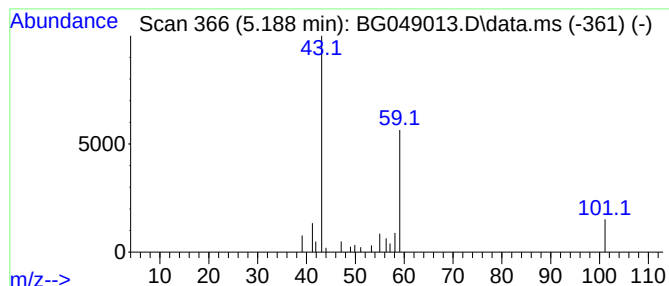
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown5.188 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.188	2.13 ng	23477	1,4-Dichlorobenzene-d4	8.114

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
4			1,2-Butanediol	90	C4H10O2	000584-03-2	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7



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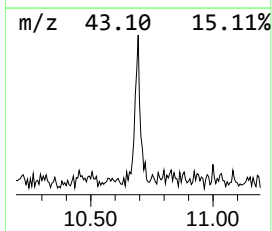
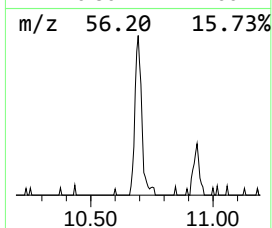
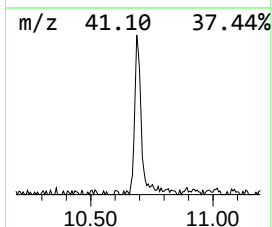
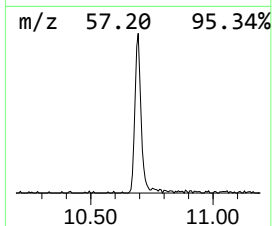
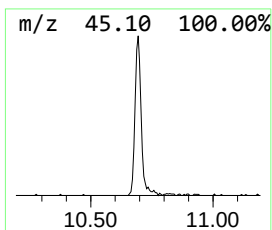
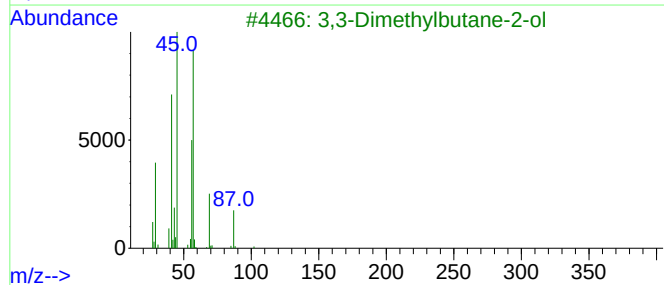
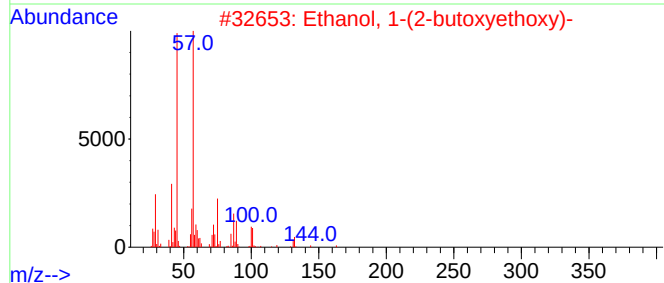
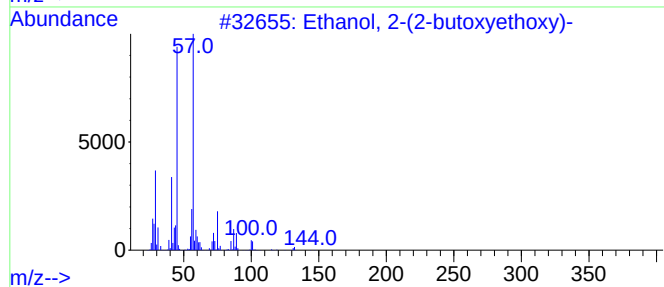
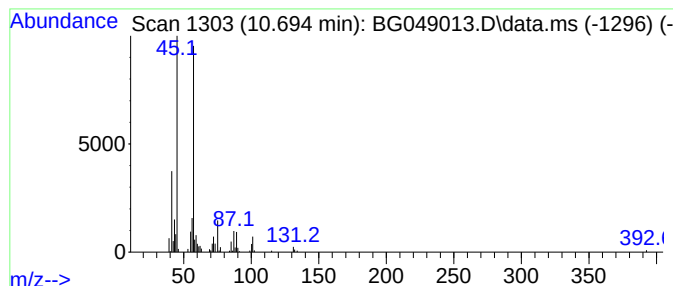
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.694	12.64 ng	179314	Naphthalene-d8	10.935

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40
4			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	40
5			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40



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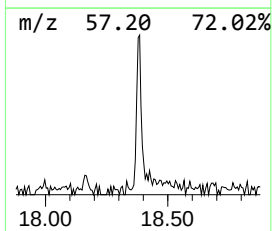
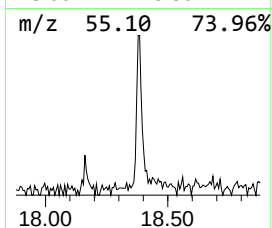
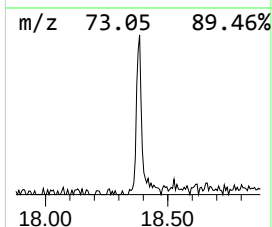
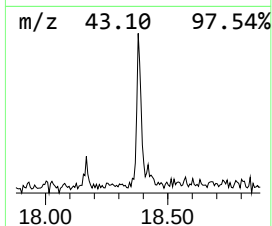
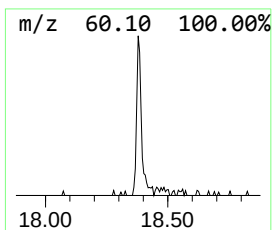
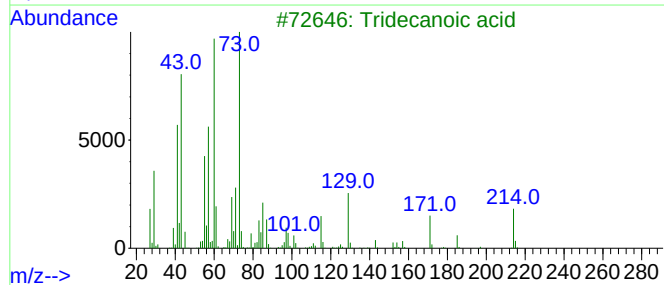
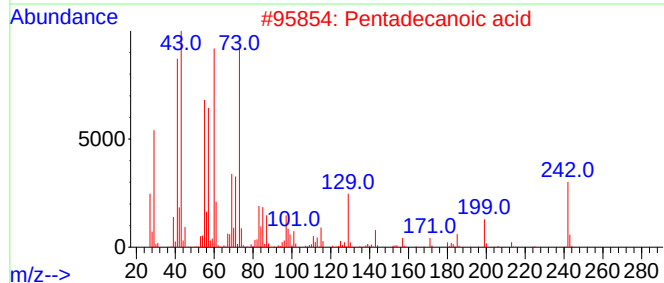
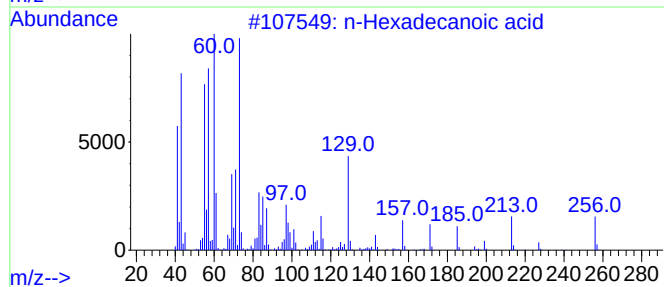
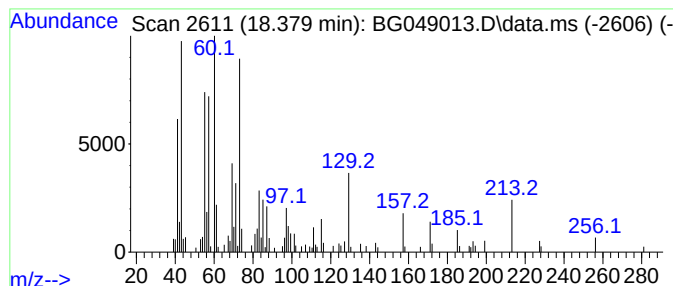
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.379	4.39 ng	121656	Phenanthrene-d10	17.503

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	78
3			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Nonanoic acid	158	C9H18O2	000112-05-0	46
5			i-Propyl 14-methyl-pentadecanoate	298	C19H38O2	1000336-62-4	43



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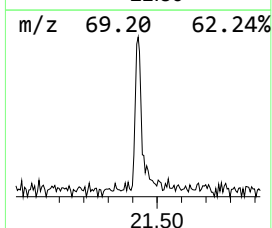
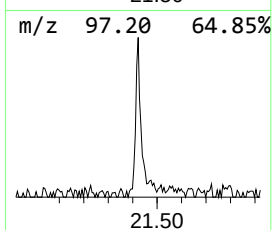
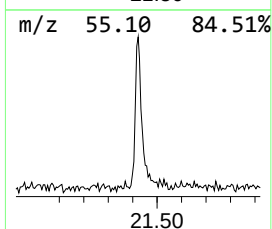
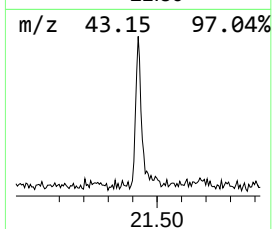
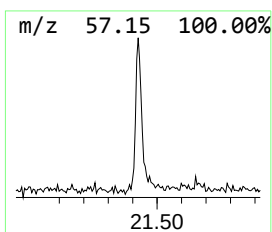
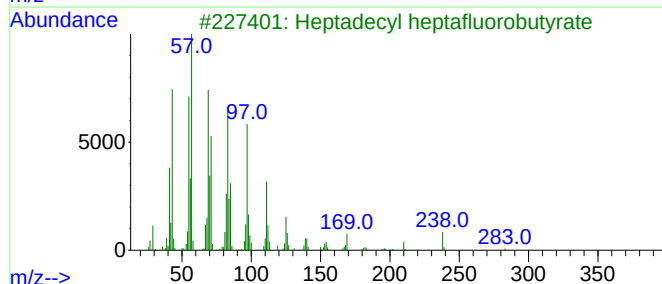
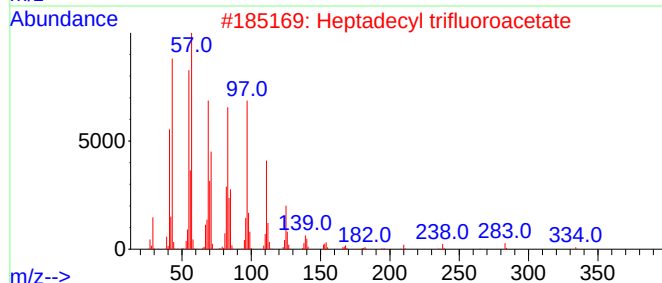
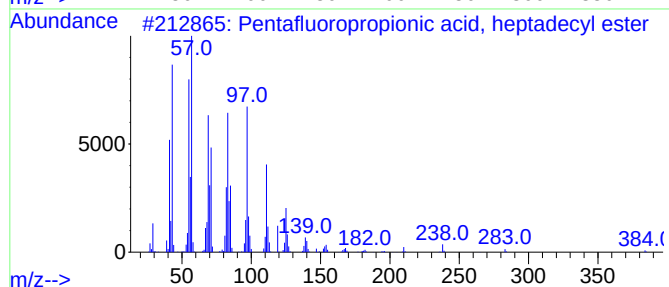
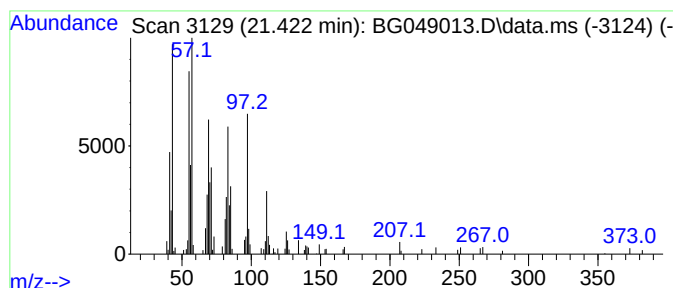
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.422	4.42 ng	137447	Chrysene-d12	21.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
4			Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	90
5			E-15-Heptadecenal	252	C17H32O	1000130-97-9	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.238	2.9	ng	31568	1	8.114	220669	20.0
unknown5.188	5.188	2.1	ng	23477	1	8.114	220669	20.0
Ethanol, 2-(2-b...	10.694	12.6	ng	179314	2	10.935	283655	20.0
n-Hexadecanoic ...	18.379	4.4	ng	121656	4	17.503	554028	20.0
Pentafluoroprop...	21.422	4.4	ng	137447	5	21.792	622623	20.0