

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111022\
 Data File : BG055552.D
 Acq On : 10 Nov 2022 23:43
 Operator : CG/JU
 Sample : N5476-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RED-006-6

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.329	3	7	23	rVB	823534	1436362	51.54%	10.680%
2	4.710	237	242	248	rBV	24848	38976	1.40%	0.290%
3	5.321	341	346	353	rBV	59210	95162	3.41%	0.708%
4	5.791	419	426	435	rBV	297737	486737	17.47%	3.619%
5	7.395	692	699	710	rVB	206116	348689	12.51%	2.593%
6	8.270	841	848	854	rBV	172531	291041	10.44%	2.164%
7	9.440	1038	1047	1056	rBV	485853	861439	30.91%	6.405%
8	11.096	1321	1329	1337	rVB	230335	414863	14.89%	3.085%
9	13.517	1733	1741	1748	rBV	1317341	2081450	74.69%	15.477%
10	14.886	1966	1974	1982	rVB	381007	588386	21.11%	4.375%
11	16.361	2218	2225	2237	rBV	849235	1281182	45.97%	9.526%
12	17.624	2434	2440	2448	rVB	506477	757308	27.18%	5.631%
13	18.488	2582	2587	2592	rBV2	51357	80498	2.89%	0.599%
14	19.745	2797	2801	2810	rBV5	31709	48473	1.74%	0.360%
15	20.209	2874	2880	2889	rBV	2108099	2786765	100.00%	20.721%
16	21.531	3101	3105	3114	rVB4	41320	66773	2.40%	0.496%
17	21.919	3165	3171	3178	rVB	521566	869642	31.21%	6.466%
18	25.339	3743	3753	3773	rVB2	294061	915311	32.84%	6.806%

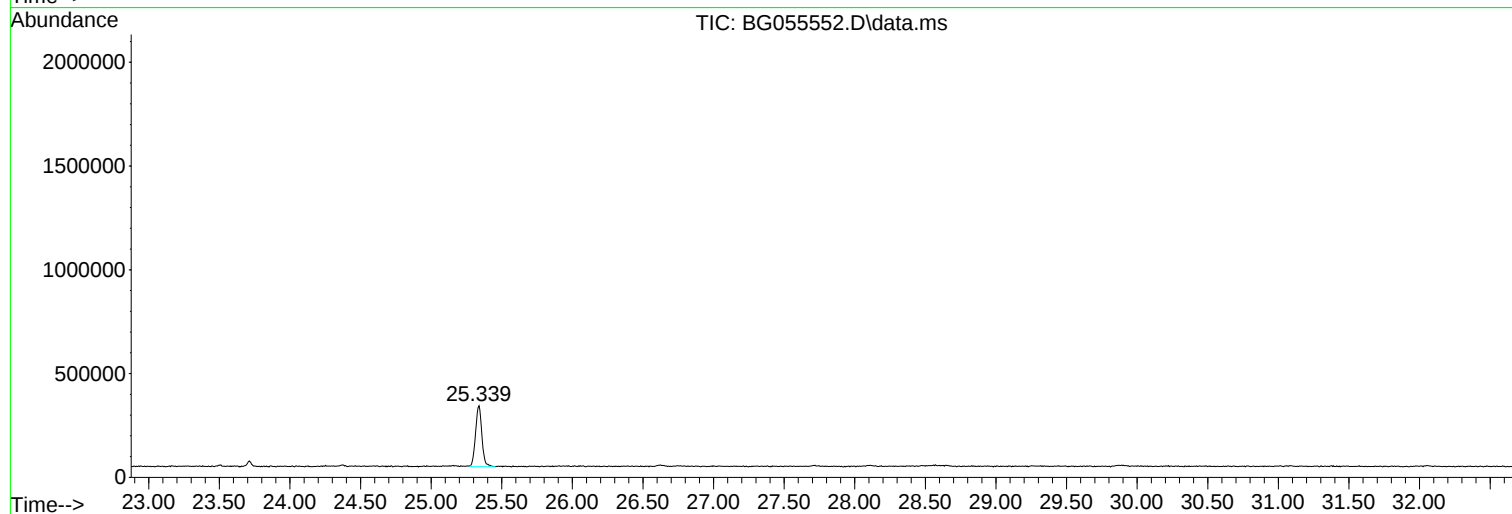
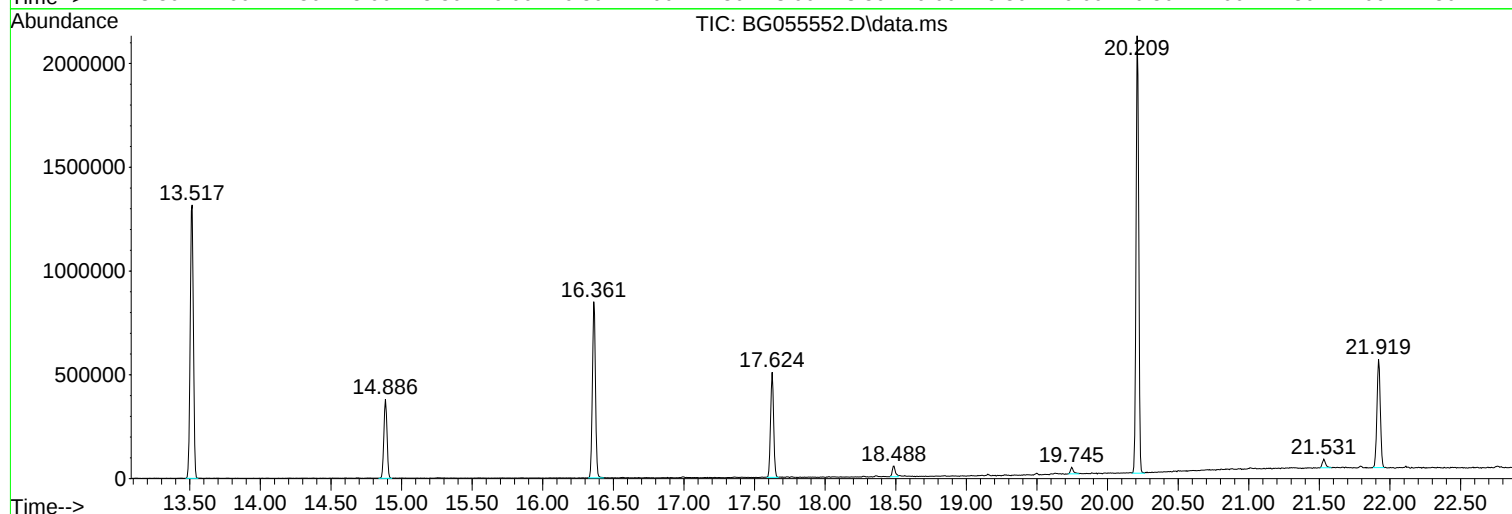
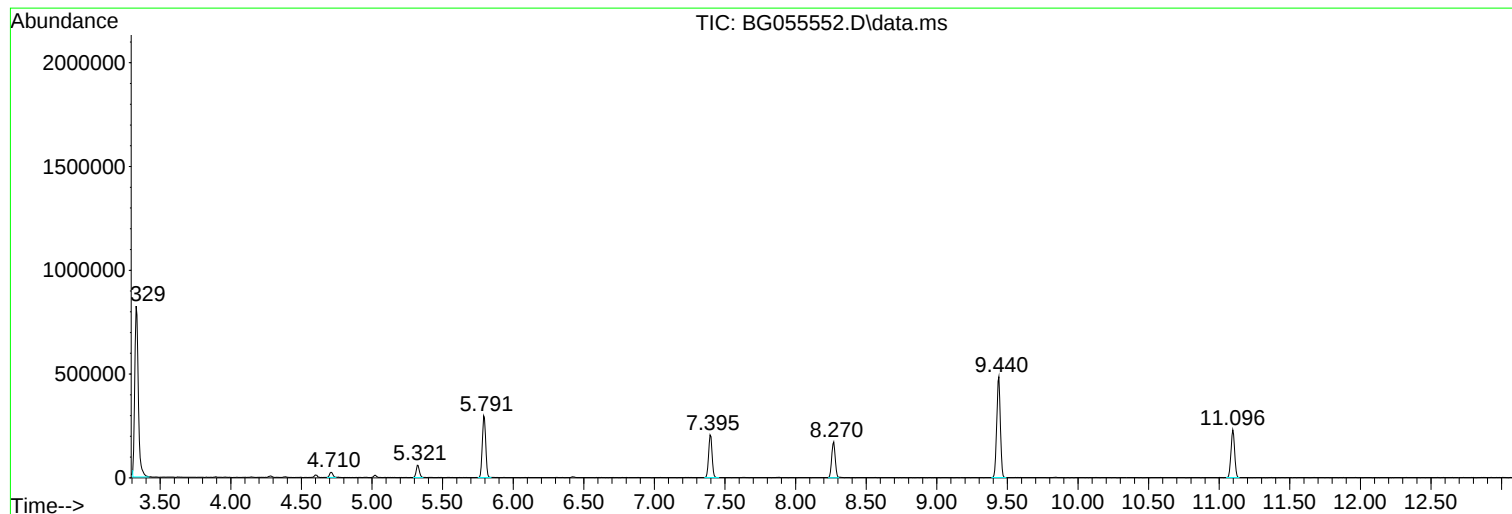
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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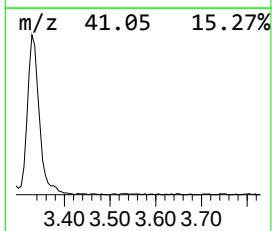
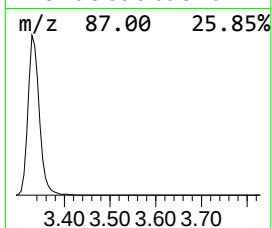
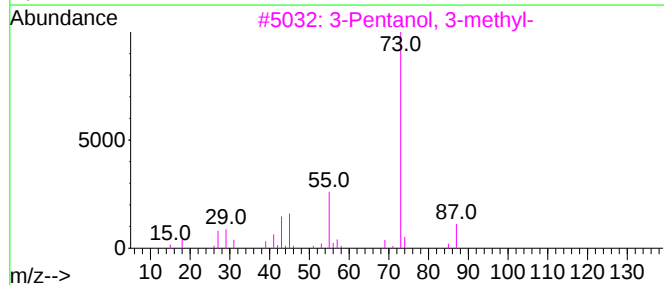
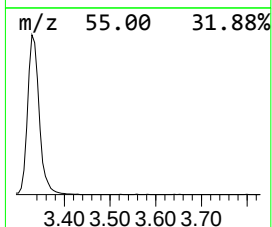
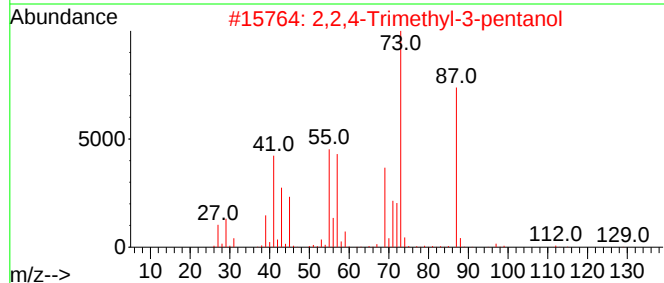
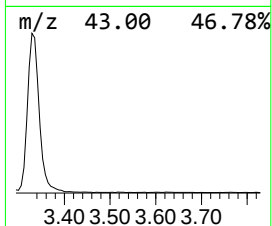
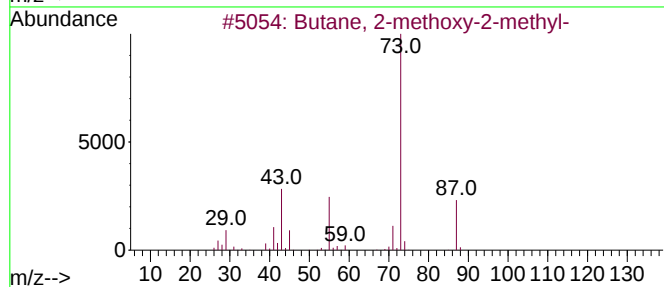
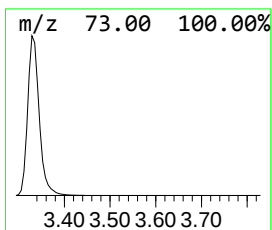
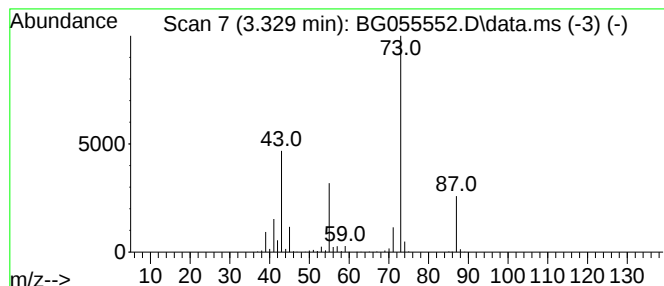
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.329	98.71 ng	1436360	1,4-Dichlorobenzene-d4	8.270

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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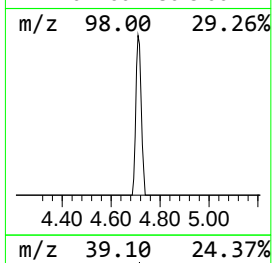
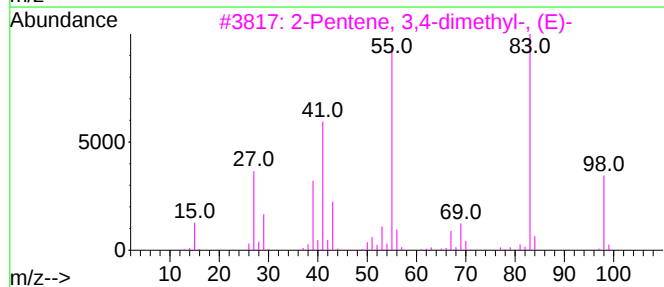
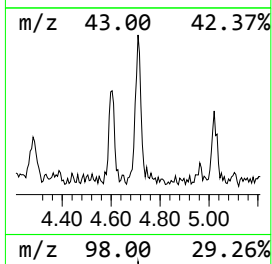
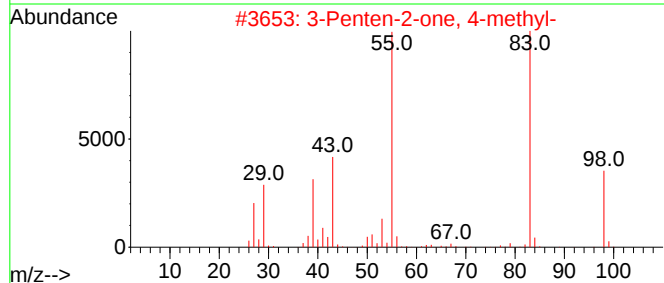
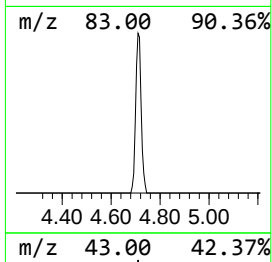
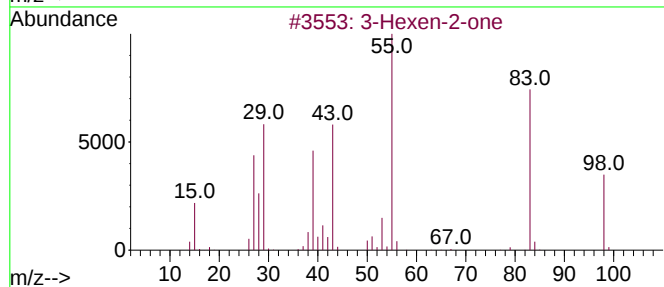
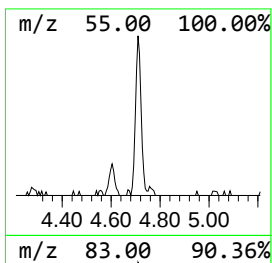
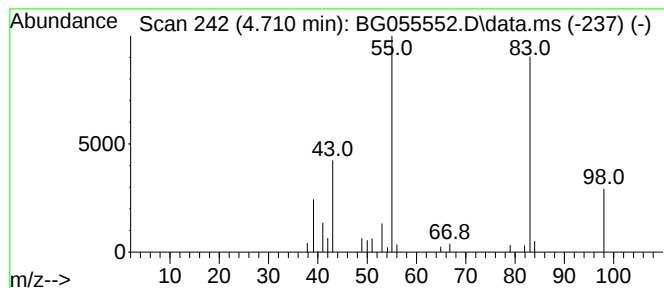
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.710	2.68 ng	38976	1,4-Dichlorobenzene-d4	8.270

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	90
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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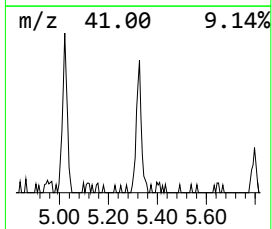
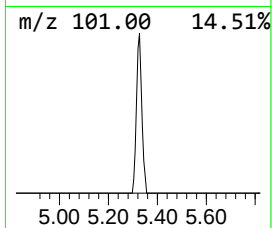
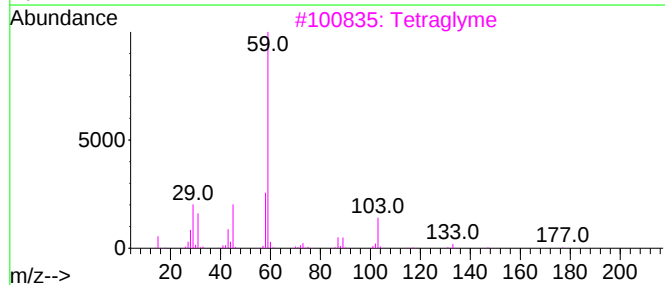
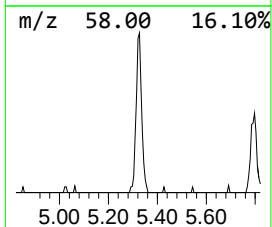
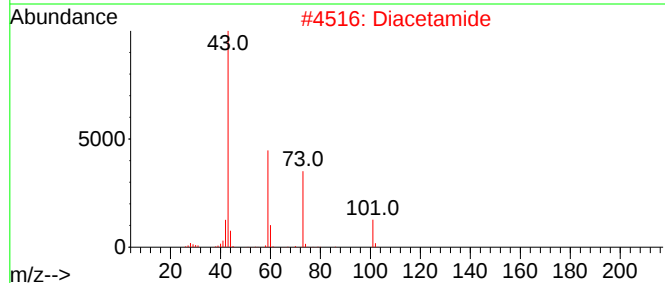
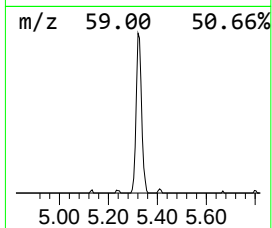
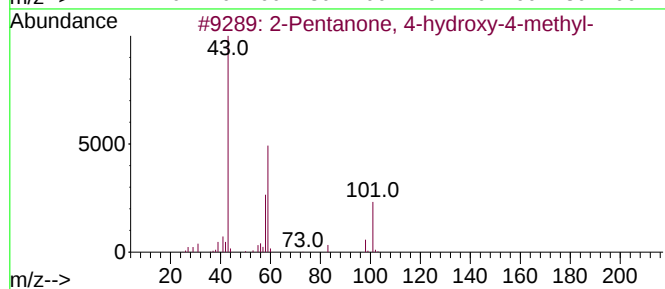
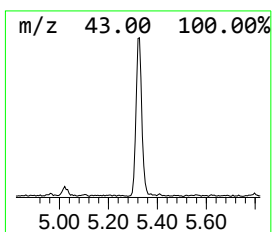
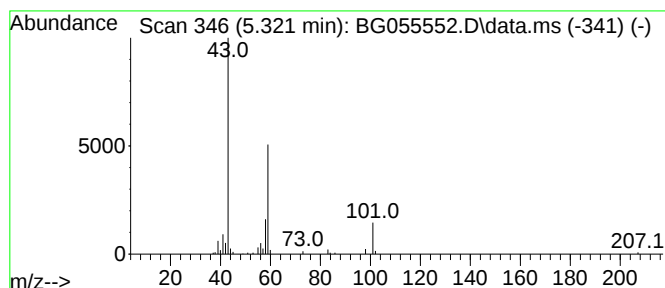
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.321	6.54 ng	95162	1,4-Dichlorobenzene-d4	8.270

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Diacetamide	101	C4H7NO2	000625-77-4	36		
3	Tetraglyme	222	C10H22O5	000143-24-8	28		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	25		



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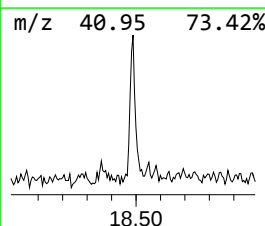
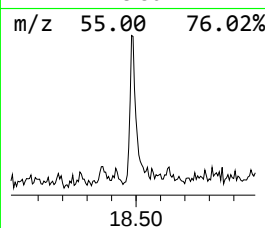
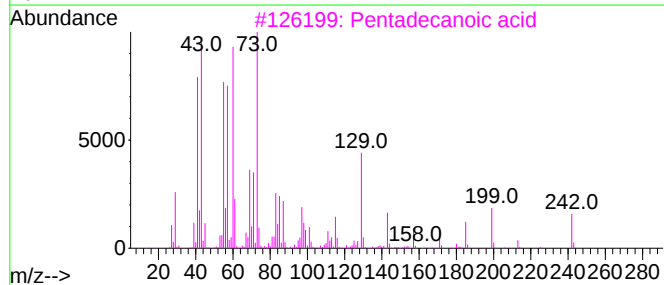
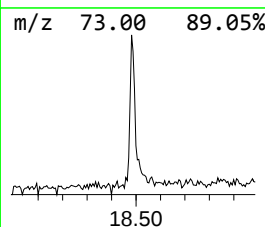
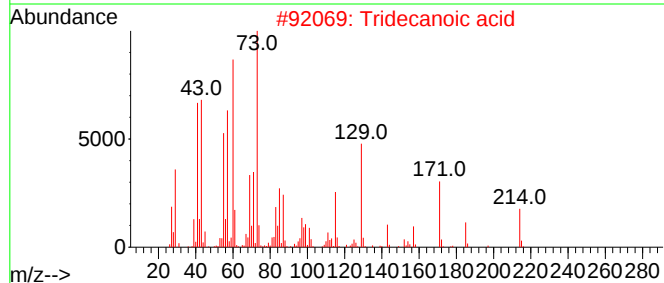
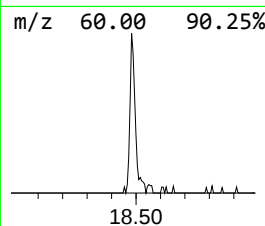
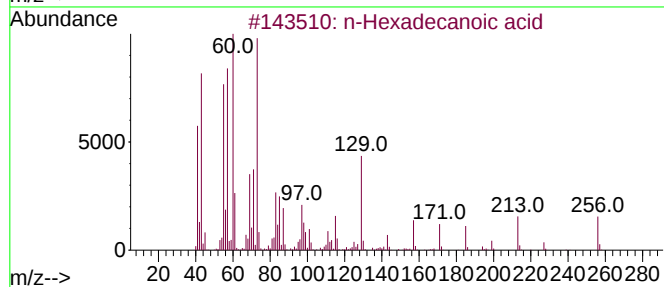
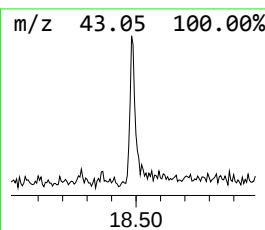
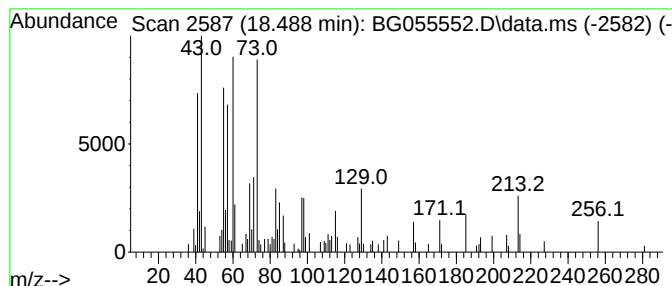
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	2.13 ng	80498	Phenanthrene-d10	17.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.329	98.7	ng	1436360	1	8.270	291041	20.0
3-Hexen-2-one	4.710	2.7	ng	38976	1	8.270	291041	20.0
2-Pentanone, 4-...	5.321	6.5	ng	95162	1	8.270	291041	20.0
n-Hexadecanoic ...	18.488	2.1	ng	80498	4	17.624	757308	20.0