

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041323\
 Data File : BG057085.D
 Acq On : 13 Apr 2023 17:09
 Operator : CG/JU
 Sample : 02293-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 IDW-LIQ-FRAC-041123

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057085.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.435	318	323	330	rVB2	12343	19101	1.51%	0.405%
2	5.917	396	405	414	rBV	137017	226499	17.96%	4.804%
3	7.533	673	680	689	rBV	86803	144333	11.45%	3.061%
4	8.402	822	828	838	rBB	56764	95222	7.55%	2.019%
5	9.583	1021	1029	1037	rVB	189352	333338	26.43%	7.069%
6	11.239	1304	1311	1319	rBV	71001	126321	10.02%	2.679%
7	13.642	1713	1720	1727	rVB	516625	776660	61.59%	16.472%
8	14.923	1930	1938	1945	rBV	20520	25538	2.03%	0.542%
9	15.011	1945	1953	1962	rVB	110907	178608	14.16%	3.788%
10	16.350	2175	2181	2187	rBV	46963	65386	5.18%	1.387%
11	16.491	2199	2205	2216	rBV	406153	629144	49.89%	13.343%
12	16.914	2271	2277	2283	rVB3	8930	13483	1.07%	0.286%
13	17.754	2413	2420	2427	rVB	155281	232124	18.41%	4.923%
14	18.588	2556	2562	2571	rBV	27561	38863	3.08%	0.824%
15	19.839	2771	2775	2784	rVB6	9527	15115	1.20%	0.321%
16	20.127	2820	2824	2829	rVB3	10260	13537	1.07%	0.287%
17	20.321	2851	2857	2863	rBV	1006755	1261097	100.00%	26.746%
18	21.631	3076	3080	3085	rBV6	13293	23186	1.84%	0.492%
19	22.072	3147	3155	3161	rBV2	142100	251683	19.96%	5.338%
20	25.602	3746	3756	3767	rVB	83406	245920	19.50%	5.216%

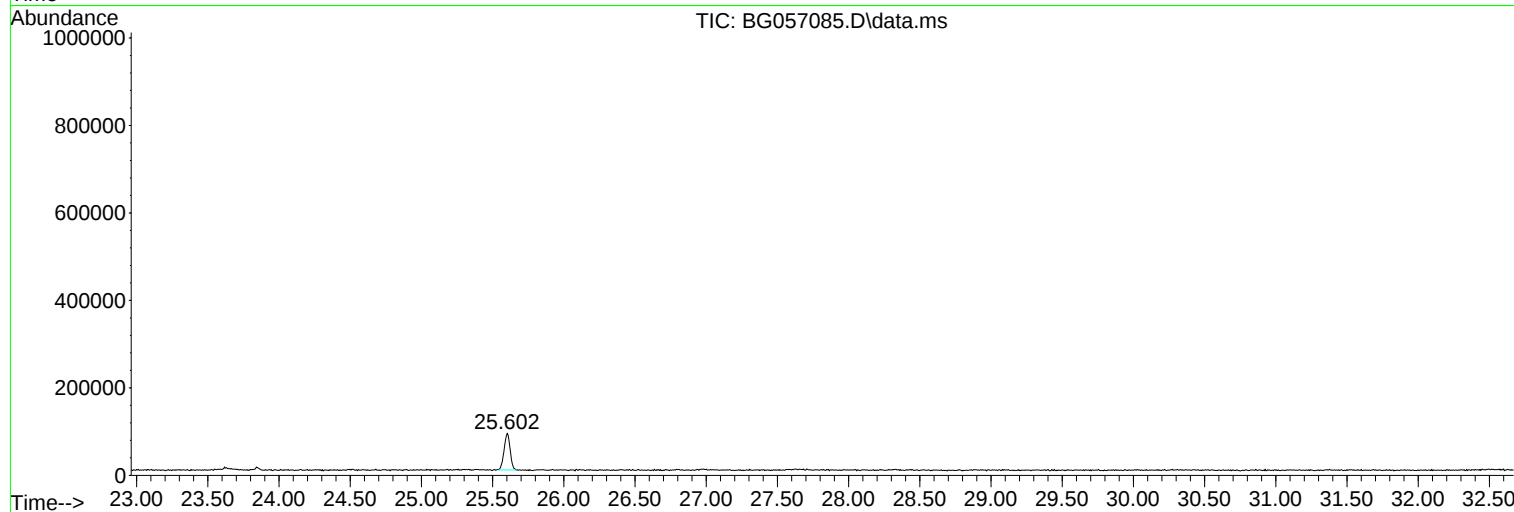
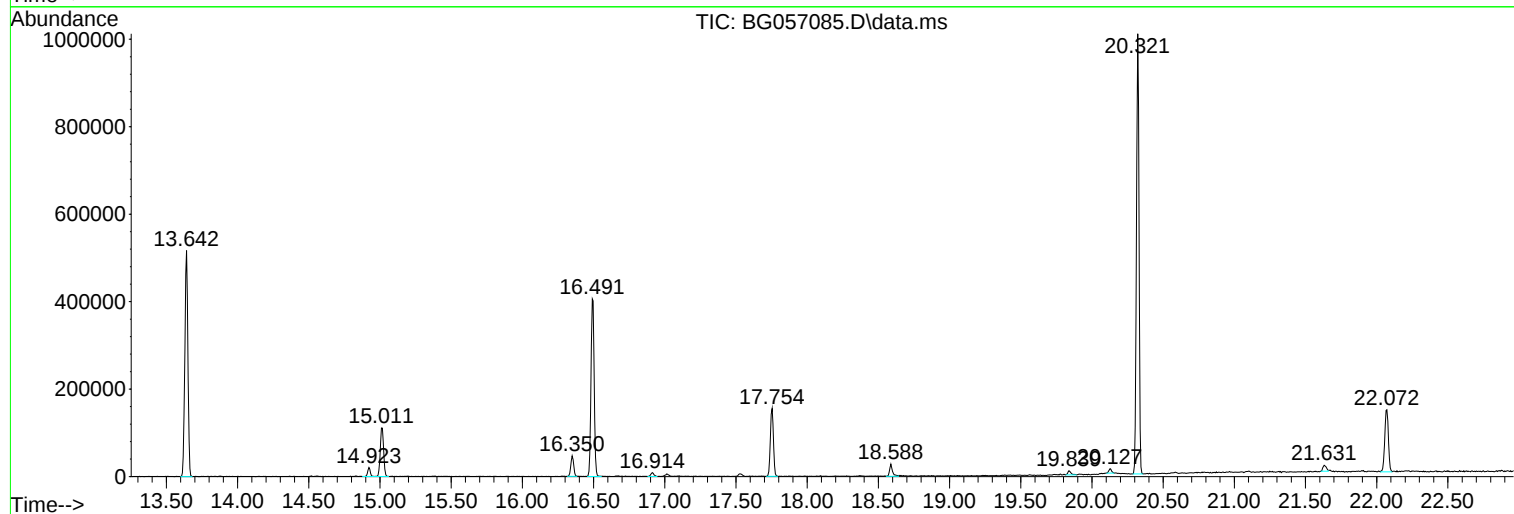
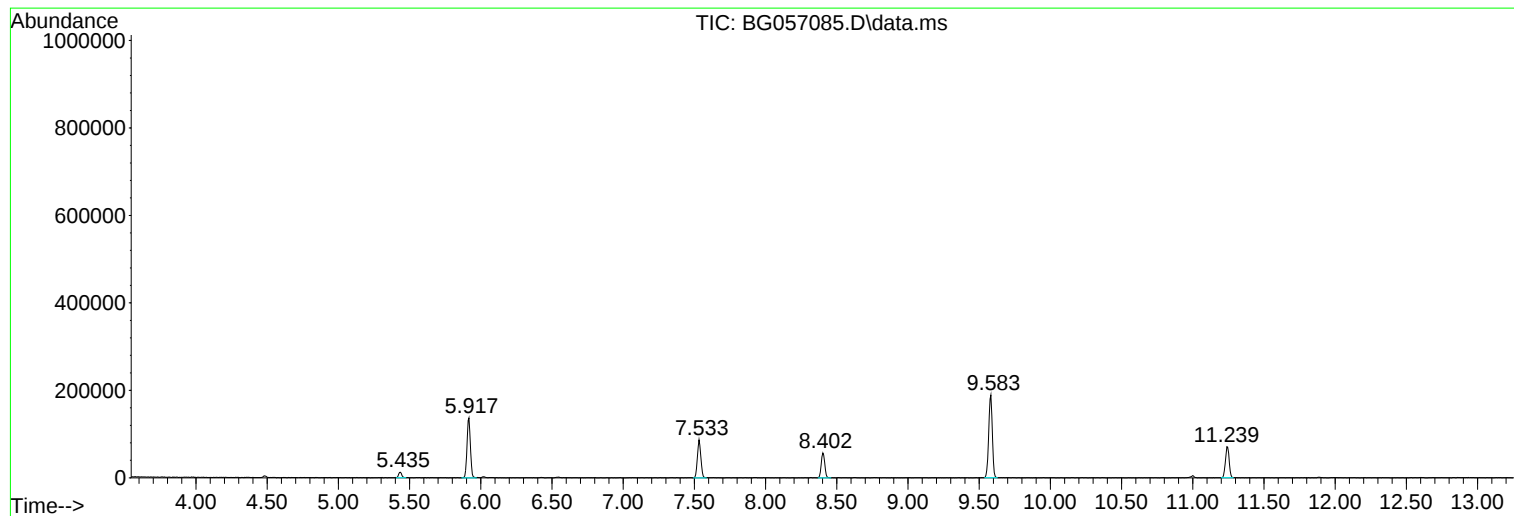
Sum of corrected areas: 4715158

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



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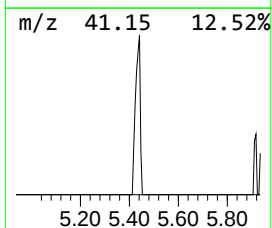
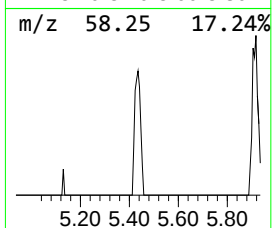
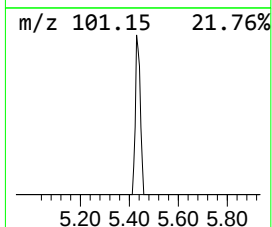
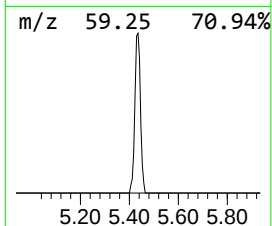
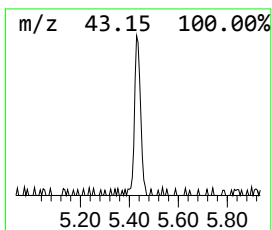
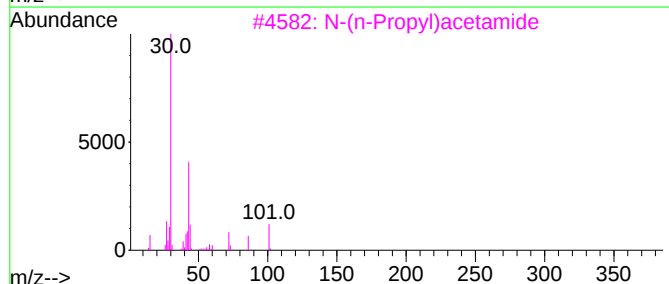
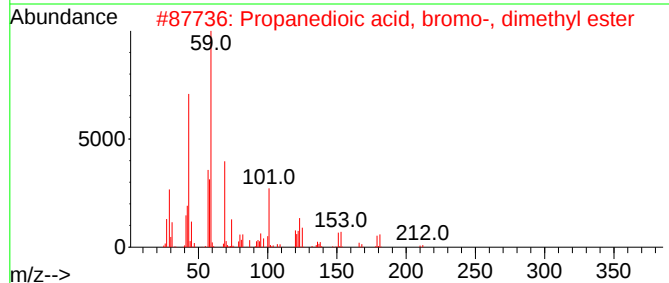
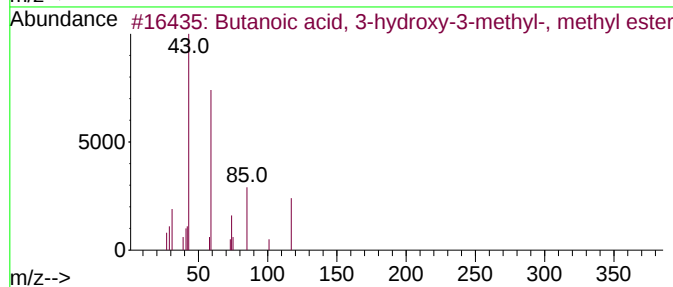
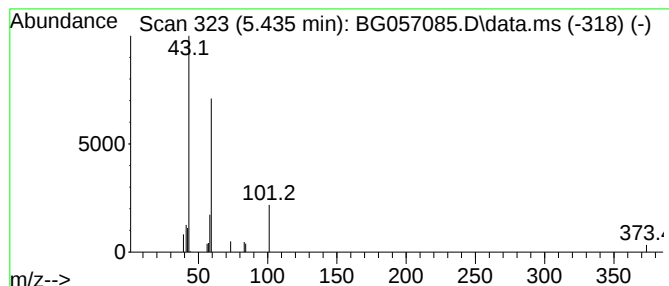
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.435 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.435	4.01 ng	19101	1,4-Dichlorobenzene-d4	8.408

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-hydroxy-3-methyl...	132	C6H12O3	006149-45-7	36
2			Propanedioic acid, bromo-, dimet...	210	C5H7BrO4	000868-26-8	33
3			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	16
4			3-Octanol	130	C8H18O	000589-98-0	9
5			Pentan-2-ol, 4-allyloxy-2-methyl-	158	C9H18O2	102840-52-8	9



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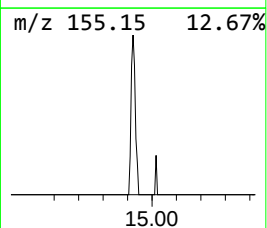
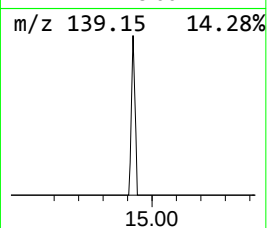
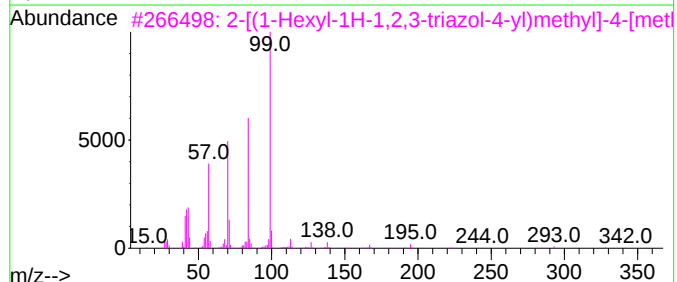
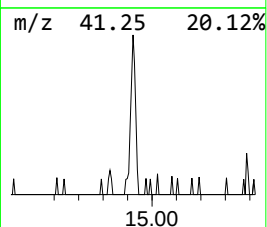
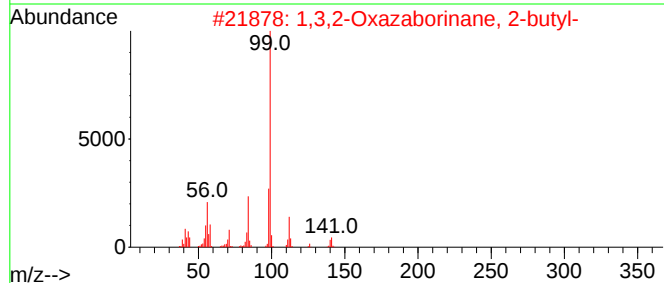
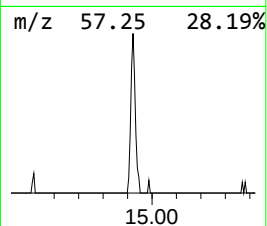
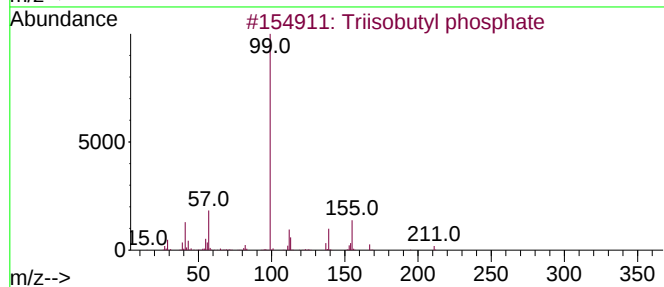
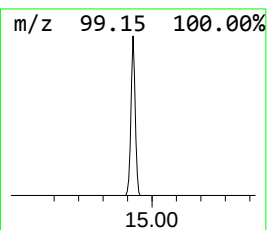
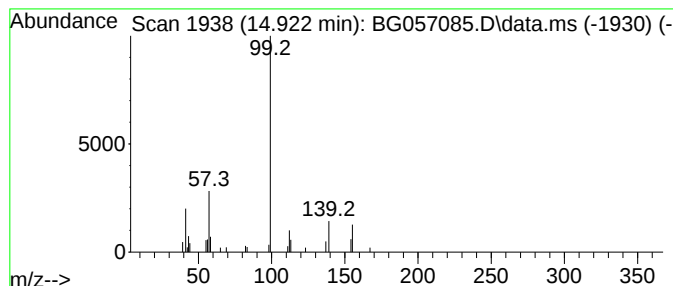
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Peak Number 2 Triisobutyl phosphate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.922	2.86 ng	25538	Acenaphthene-d10	15.017

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triisobutyl phosphate	266	C12H27O4P	000126-71-6	90
2		1,3,2-Oxazaborinane, 2-butyl-	141	C7H16BNO	024372-00-7	36
3		2-[(1-Hexyl-1H-1,2,3-triazol-4-y...	357	C16H31N5O2S	1333142-61-2	33
4		5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	9
5		2-Piperidinone	99	C5H9NO	000675-20-7	9



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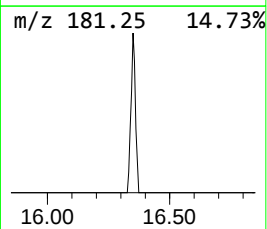
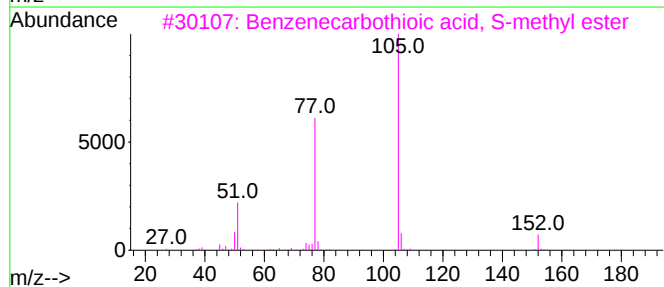
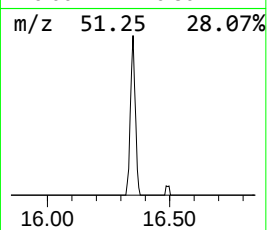
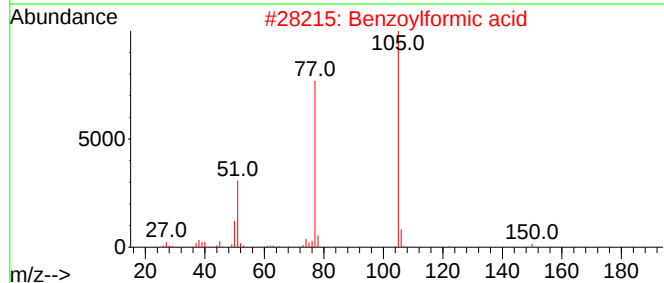
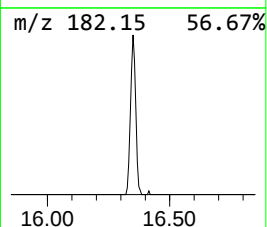
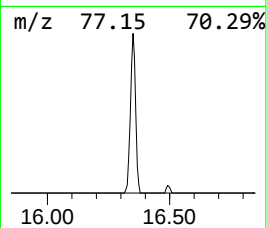
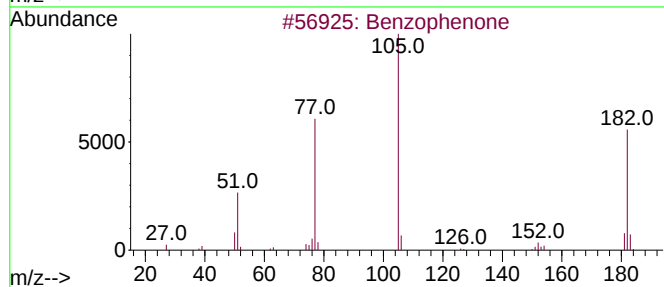
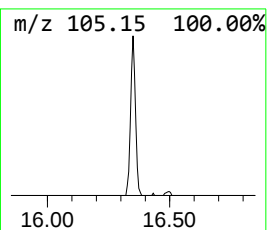
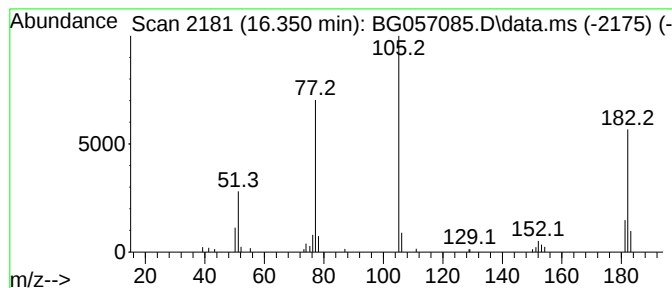
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Peak Number 3 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.350	7.32 ng	65386	Acenaphthene-d10	15.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoylformic acid	150	C8H6O3	000611-73-4	49
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
4			4,5-Diphenyloxazolin-2(3H)-one	237	C15H11NO2	005014-83-5	43
5			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	43



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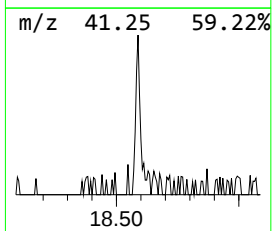
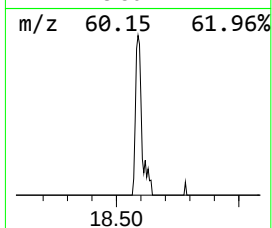
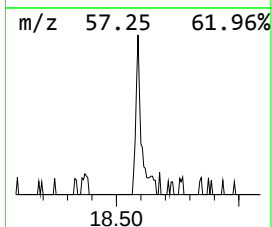
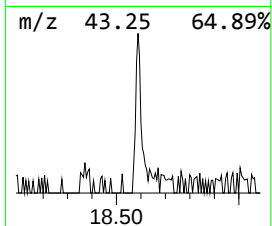
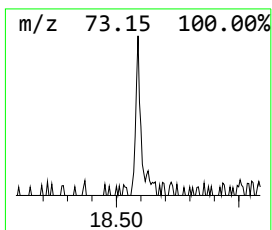
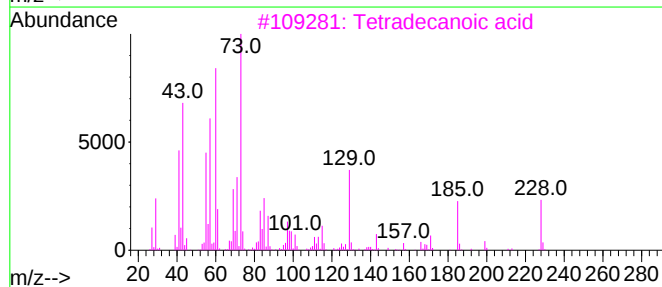
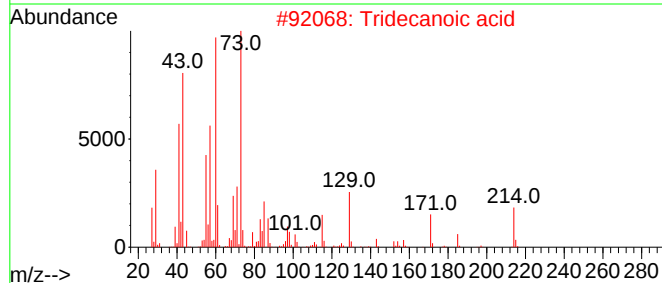
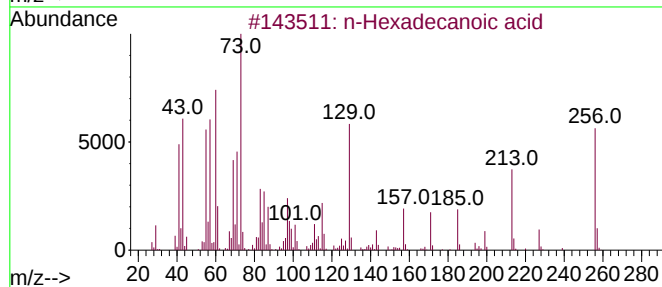
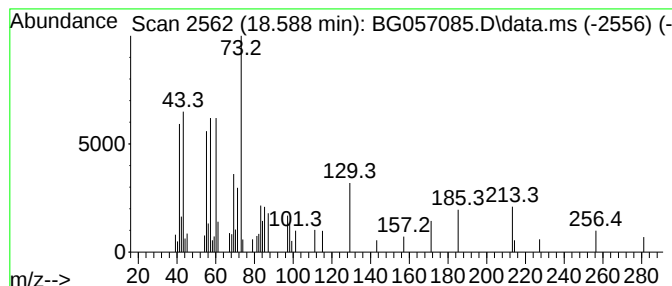
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.588	3.35 ng	38863	Phenanthrene-d10	17.754

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	55
5			Undecanoic acid	186	C11H22O2	000112-37-8	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Triisobutyl pho...	14.922	2.9	ng	25538	3	15.017	178608	20.0
Benzophenone	16.350	7.3	ng	65386	3	15.017	178608	20.0
n-Hexadecanoic ...	18.588	3.4	ng	38863	4	17.754	232124	20.0