

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102919\
 Data File : BG043377.D
 Acq On : 29 Oct 2019 17:02
 Operator : JU
 Sample : K5545-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C-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-BG102119.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.193	13	18	31	rVB	125530	198566	7.83%	1.405%
2	5.126	341	347	362	rBV	98454	165215	6.51%	1.169%
3	5.614	423	430	445	rBV	475045	866815	34.16%	6.134%
4	7.212	694	702	720	rBV	513992	1018866	40.16%	7.210%
5	7.564	754	762	776	rBV	564007	1007522	39.71%	7.129%
6	8.023	831	840	849	rBV2	136643	239839	9.45%	1.697%
7	8.346	888	895	906	rBV	419588	758958	29.91%	5.371%
8	9.186	1030	1038	1049	rBV	286193	586787	23.13%	4.152%
9	10.831	1310	1318	1330	rBV	145209	317180	12.50%	2.244%
10	13.275	1726	1734	1749	rBV	875330	1483598	58.47%	10.498%
11	14.104	1869	1875	1888	rBV	95069	186772	7.36%	1.322%
12	14.650	1962	1968	1984	rBV	302873	511336	20.15%	3.618%
13	16.137	2212	2221	2241	rBV	750046	1391362	54.84%	9.846%
14	17.394	2428	2435	2447	rBV2	362887	647792	25.53%	4.584%
15	17.512	2451	2455	2462	rVB5	23463	38799	1.53%	0.275%
16	18.287	2582	2587	2598	rBV6	34262	81817	3.22%	0.579%
17	20.003	2873	2879	2890	rBV	1917627	2537168	100.00%	17.953%
18	21.301	3098	3100	3112	rVB10	33358	85893	3.39%	0.608%
19	21.660	3155	3161	3171	rBV	435333	785487	30.96%	5.558%
20	22.447	3292	3295	3301	rVB5	29953	46217	1.82%	0.327%
21	23.140	3408	3413	3419	rVB3	42146	74380	2.93%	0.526%
22	23.322	3442	3444	3452	rVB4	25913	42073	1.66%	0.298%
23	23.933	3543	3548	3553	rVB6	39060	80651	3.18%	0.571%
24	24.856	3696	3705	3720	rVB2	302400	912515	35.97%	6.457%
25	25.978	3891	3896	3908	rVB6	22266	66295	2.61%	0.469%

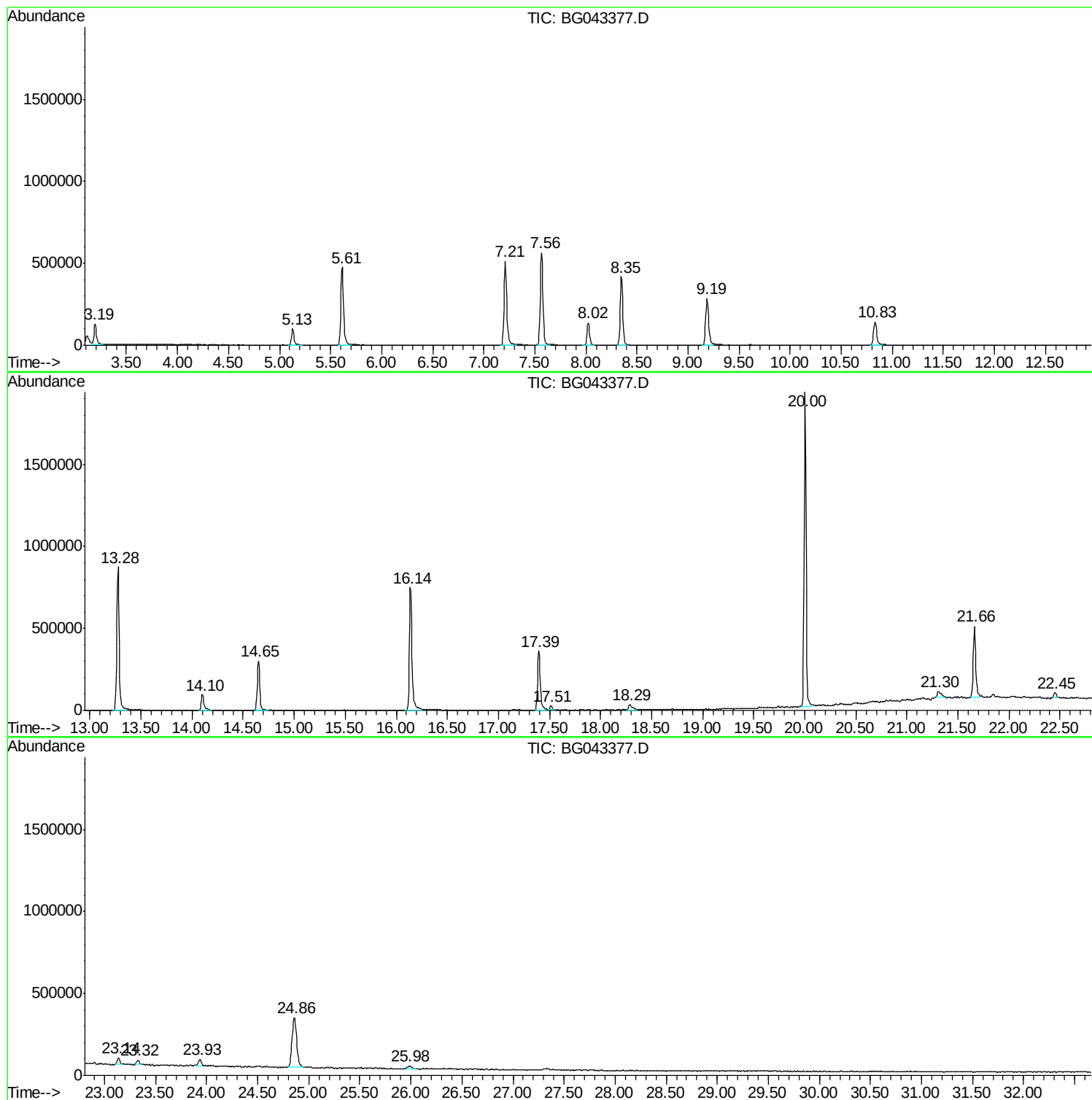
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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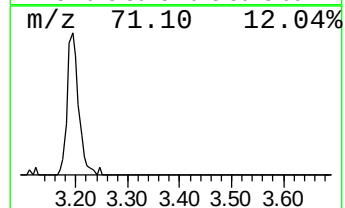
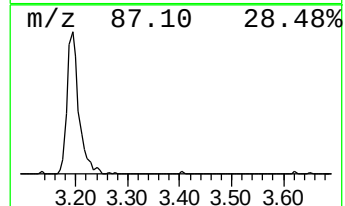
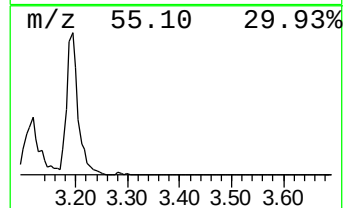
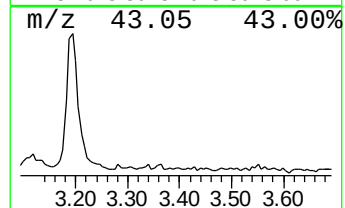
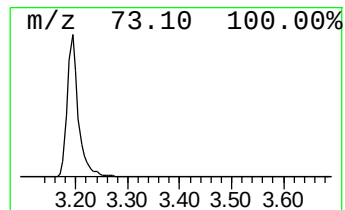
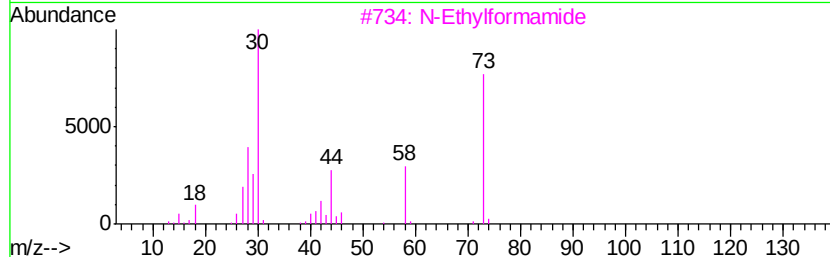
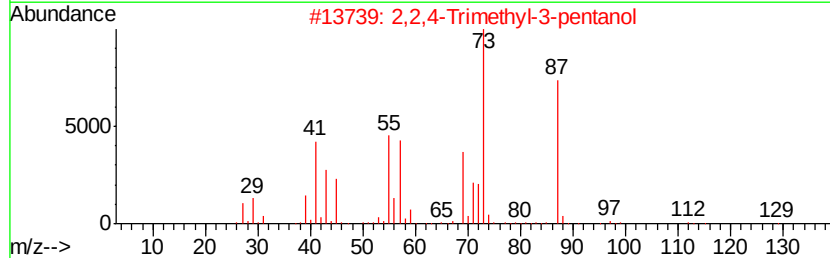
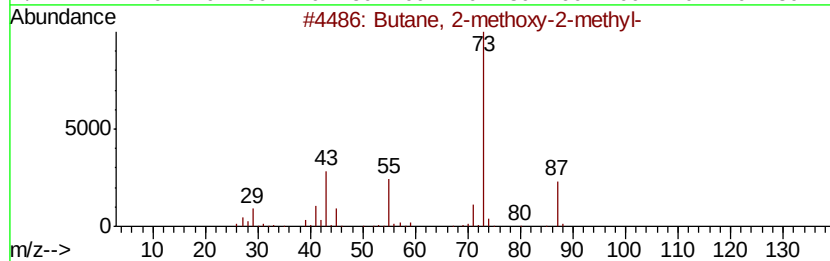
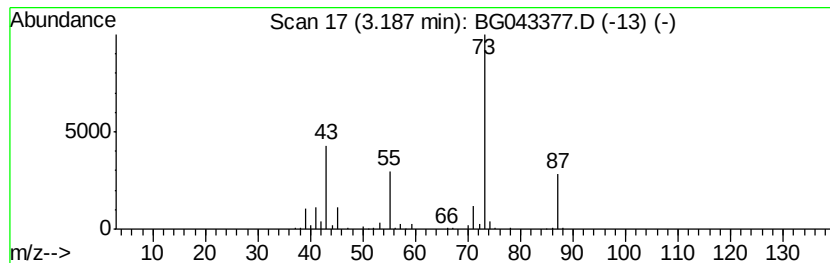
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	16.56 ng	198566	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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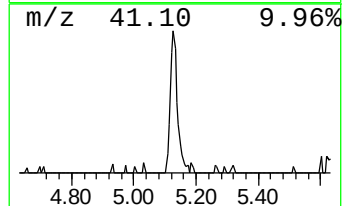
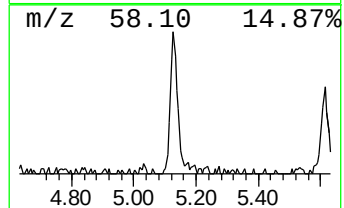
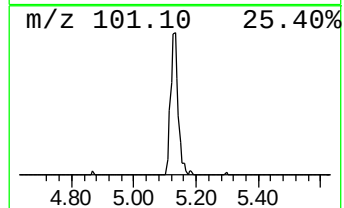
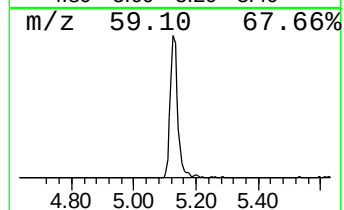
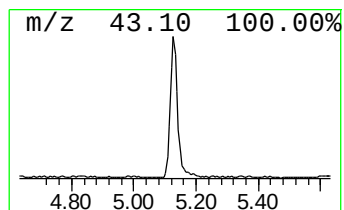
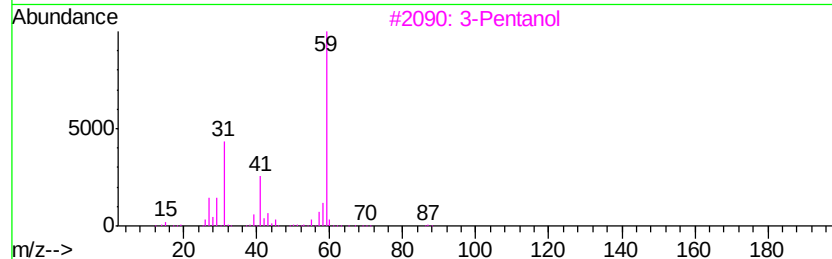
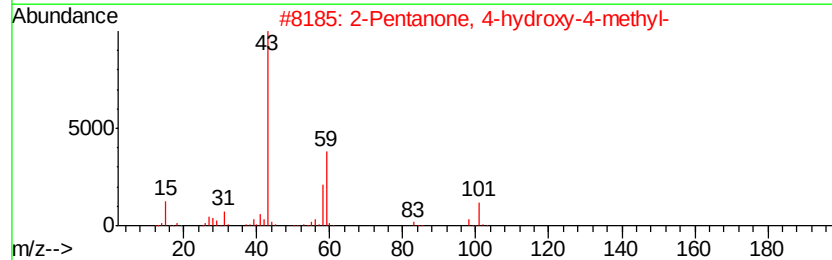
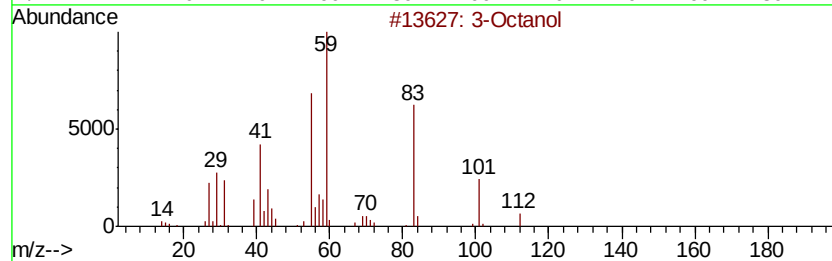
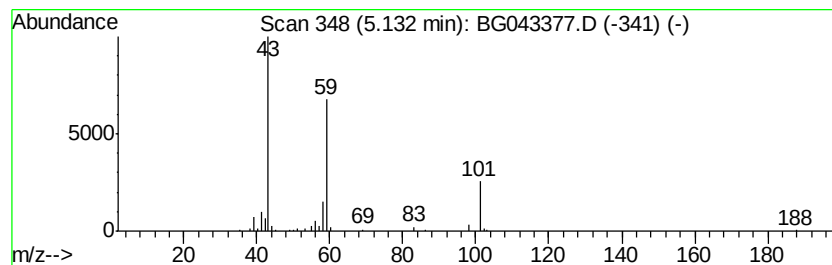
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 2 unknown5.13 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	13.78 ng	165215	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Octanol	130	C8H18O	000589-98-0	36
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
3		3-Pentanol	88	C5H12O	000584-02-1	32
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12



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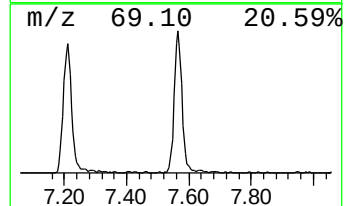
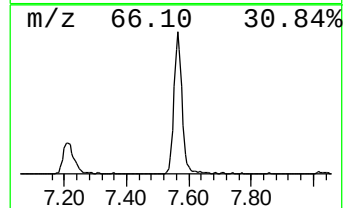
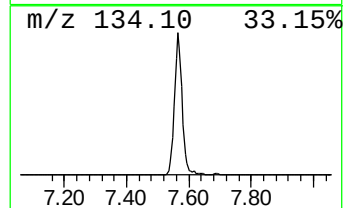
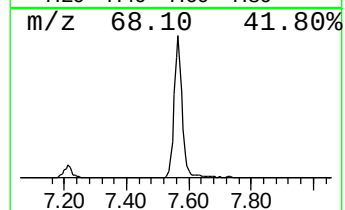
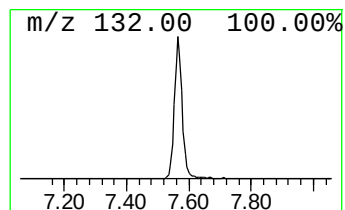
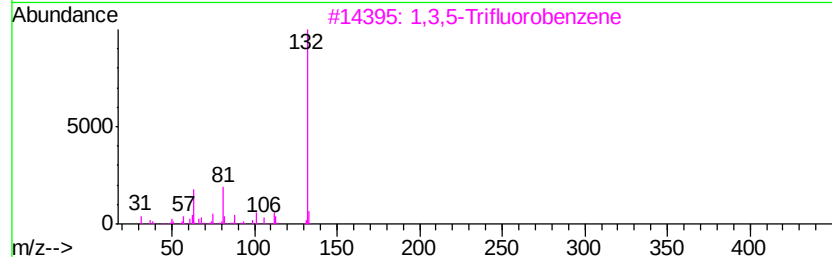
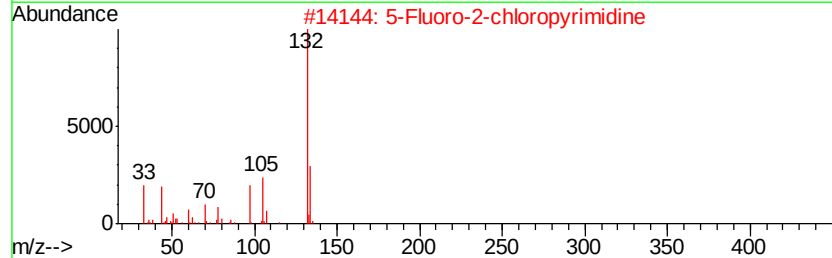
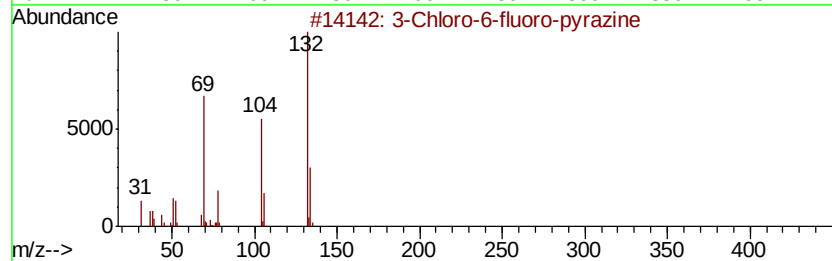
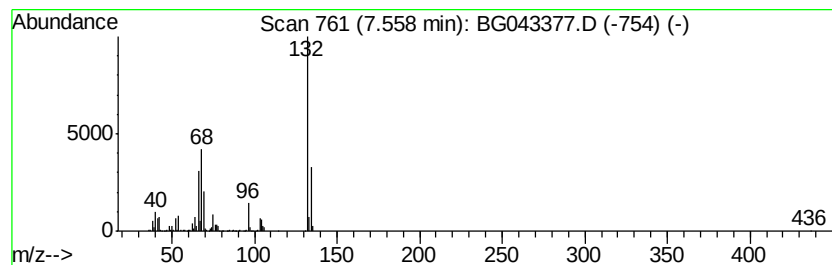
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Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	84.02 ng	1007520	1,4-Dichlorobenzene-d4	8.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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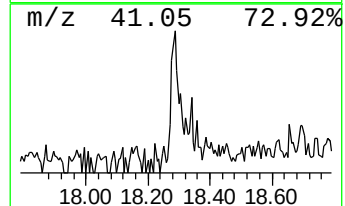
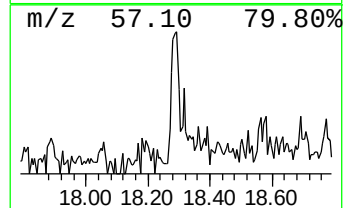
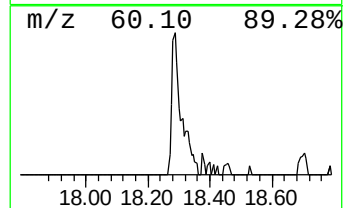
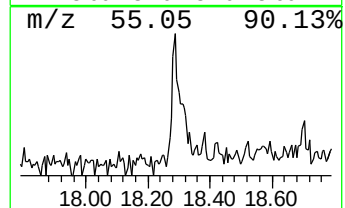
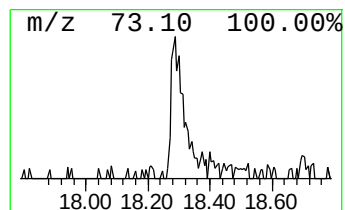
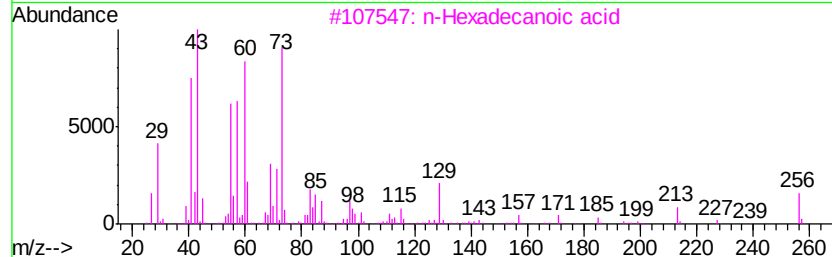
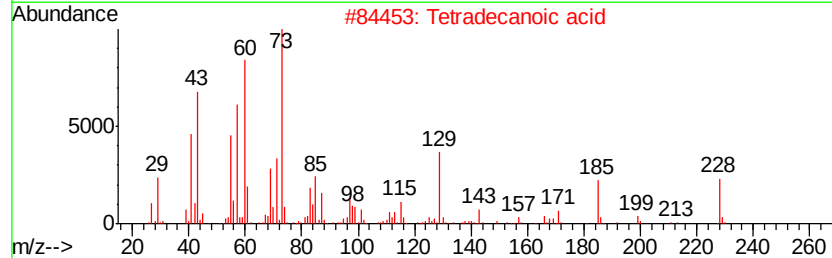
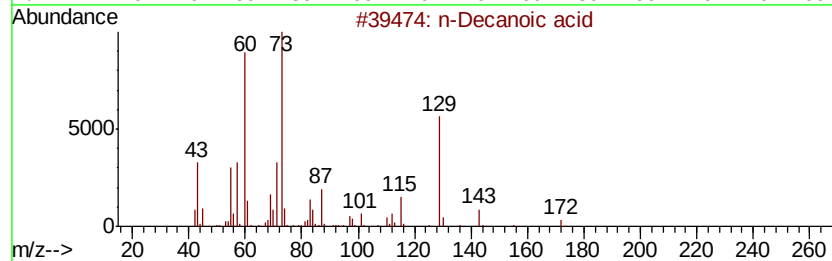
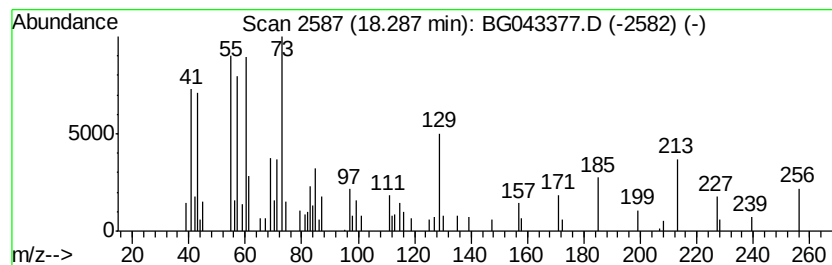
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Peak Number 5 n-Decanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.29	2.53 ng	81817	Phenanthrene-d10	17.39	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4	Lactose	342	C12H22O11	000063-42-3	43
5	Undecanoic acid	186	C11H22O2	000112-37-8	43



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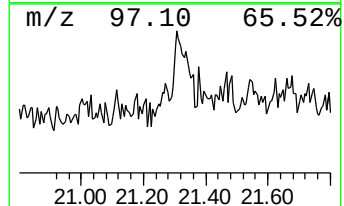
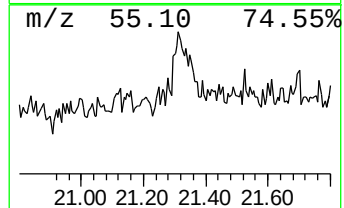
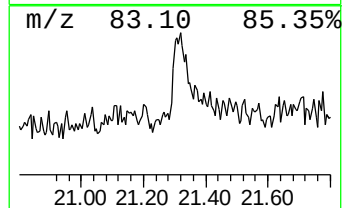
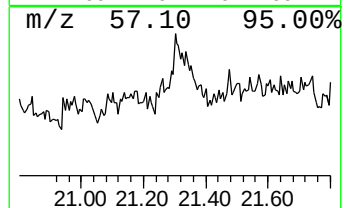
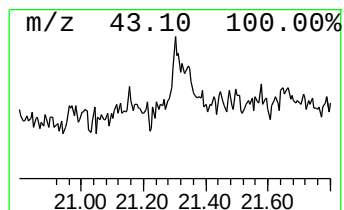
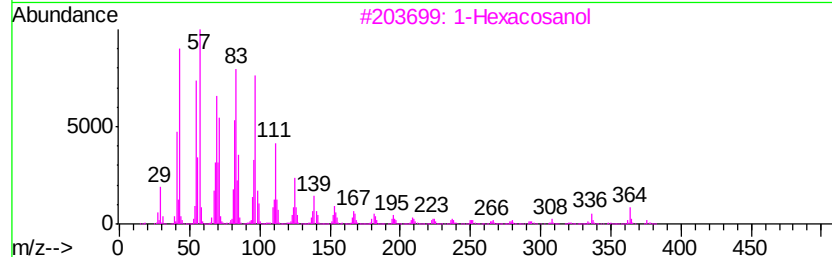
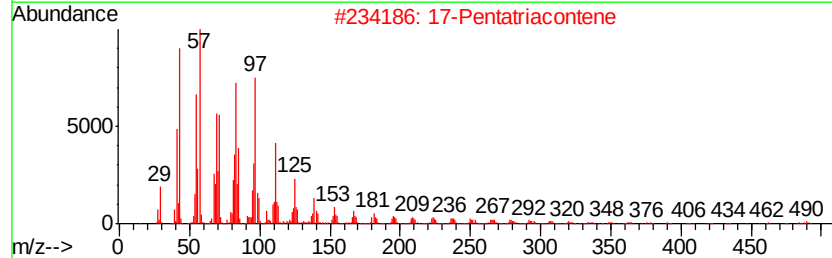
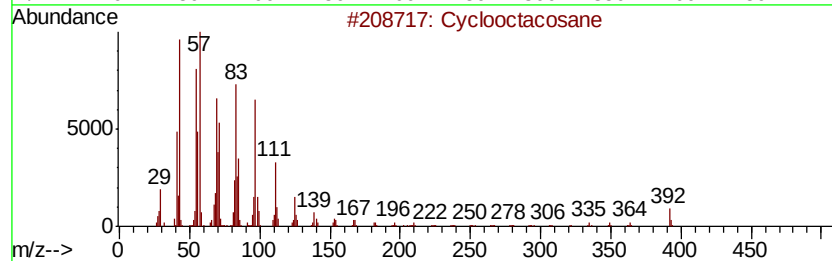
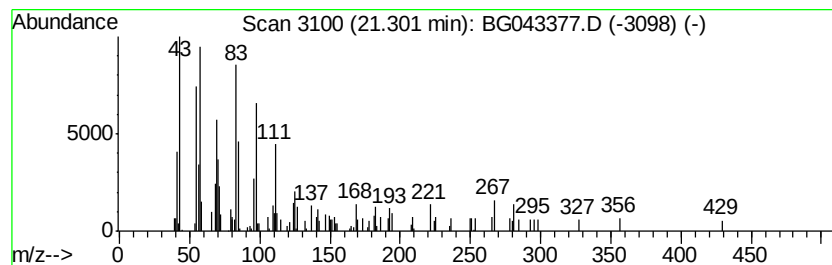
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Peak Number 6 Cyclooctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	2.19 ng	85893	Chrysene-d12	21.66
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclooctacosane	392 C28H56	000297-24-5 80
2		17-Pentatriacontene	491 C35H70	006971-40-0 80
3		1-Hexacosanol	382 C26H54O	000506-52-5 72
4		1-Hentetracontanol	593 C41H84O	040710-42-7 72
5		Octacosanol	410 C28H58O	000557-61-9 64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.19	16.6	ng	198566	1	8.02	239839	20.0
unknown5.13	5.13	13.8	ng	165215	1	8.02	239839	20.0
unknown7.56	7.56	84.0	ng	1007520	1	8.02	239839	20.0
n-Decanoic acid	18.29	2.5	ng	81817	4	17.39	647792	20.0
Cyclooctacosane	21.30	2.2	ng	85893	5	21.66	785487	20.0