

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092717\
 Data File : BG028958.D
 Acq On : 28 Sep 2017 1:03
 Operator : SJ/JU
 Sample : I5453-11
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TW-2-092517

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:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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	5.380	301	305	313	rBV	38759	61317	1.42%	0.389%
2	5.844	377	384	399	rBV	292821	536624	12.39%	3.406%
3	7.437	648	655	666	rBV	183563	348495	8.05%	2.212%
4	7.813	711	719	733	rBV	555305	989942	22.86%	6.284%
5	8.277	792	798	805	rBV	116573	202495	4.68%	1.285%
6	8.606	845	854	863	rBV2	495076	897487	20.73%	5.697%
7	9.452	990	998	1010	rBV	408688	785921	18.15%	4.989%
8	11.097	1272	1278	1291	rVB	152759	291532	6.73%	1.850%
9	13.518	1680	1690	1699	rBV	1297919	2100056	48.50%	13.330%
10	14.893	1918	1924	1936	rVB	271412	459738	10.62%	2.918%
11	15.286	1986	1991	2000	rBV2	93905	169602	3.92%	1.077%
12	15.615	2042	2047	2057	rVB2	40699	61179	1.41%	0.388%
13	16.385	2171	2178	2193	rBV	1327216	2118344	48.92%	13.446%
14	17.648	2384	2393	2400	rBV2	456229	719930	16.63%	4.570%
15	20.233	2827	2833	2845	rBV	3225218	4329869	100.00%	27.484%
16	21.967	3121	3128	3135	rBV	500936	868255	20.05%	5.511%
17	25.422	3704	3716	3729	rBV3	258415	813591	18.79%	5.164%

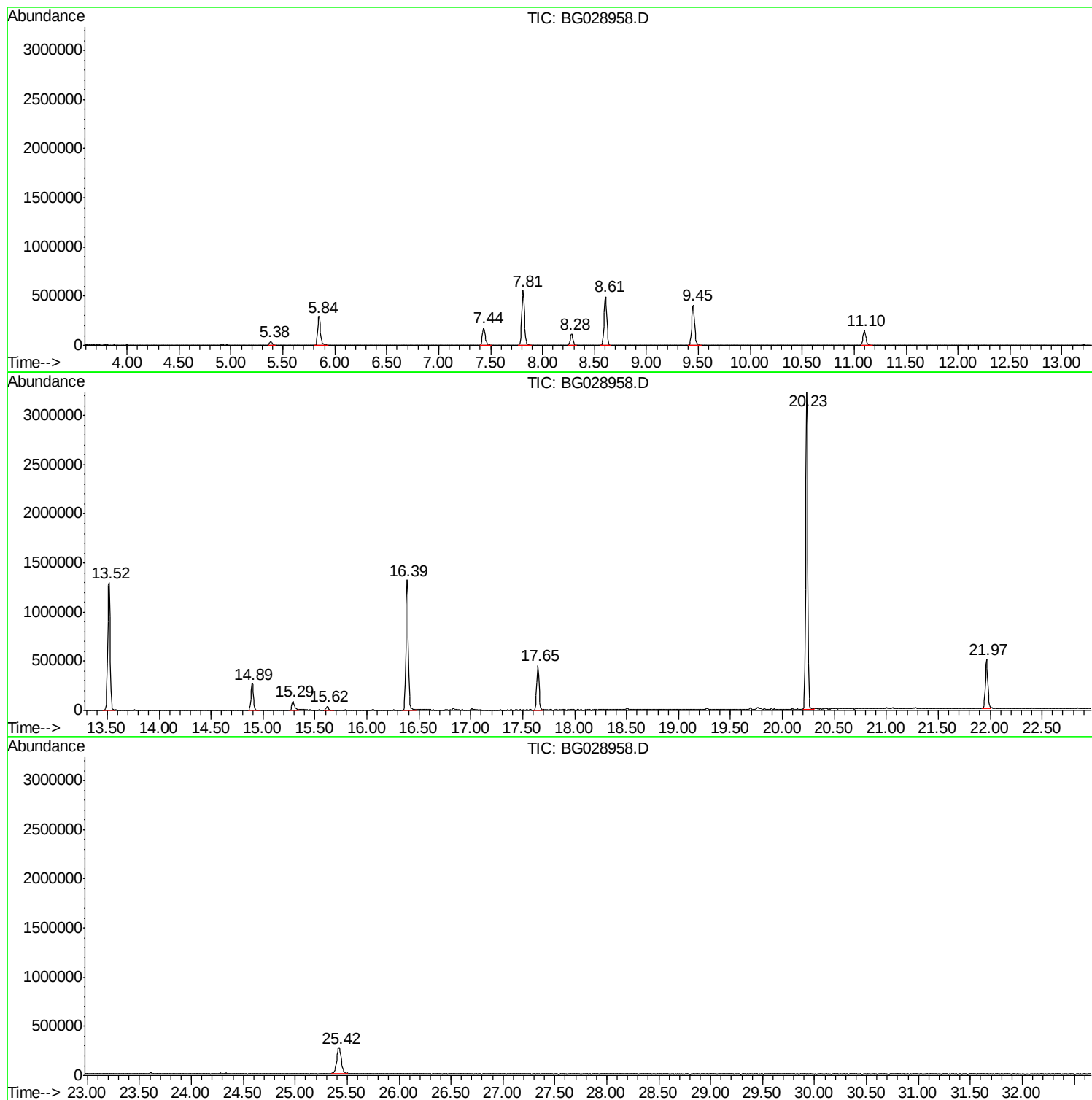
Sum of corrected areas: 15754377

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.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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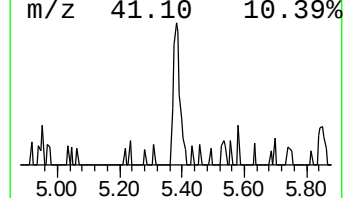
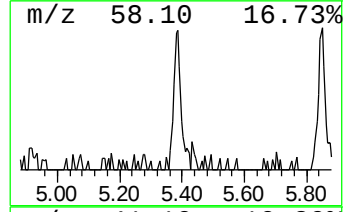
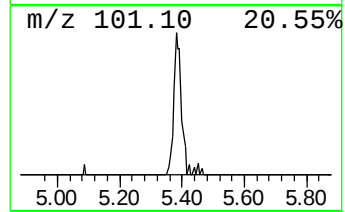
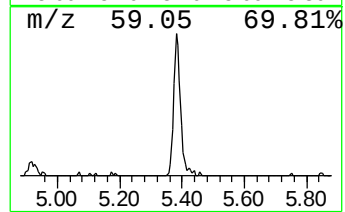
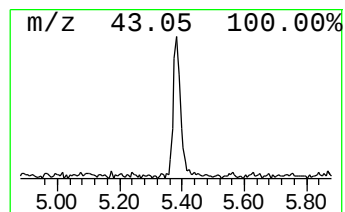
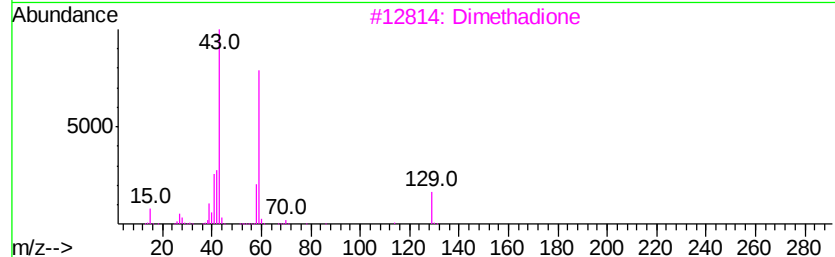
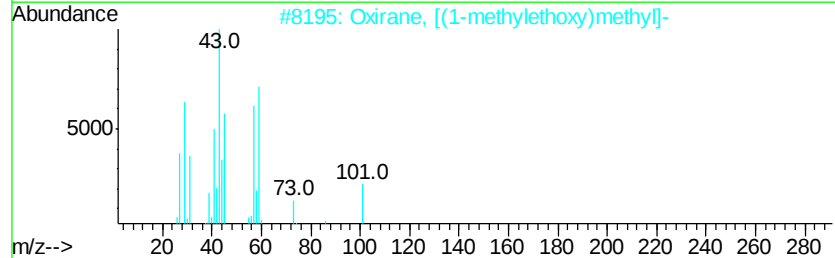
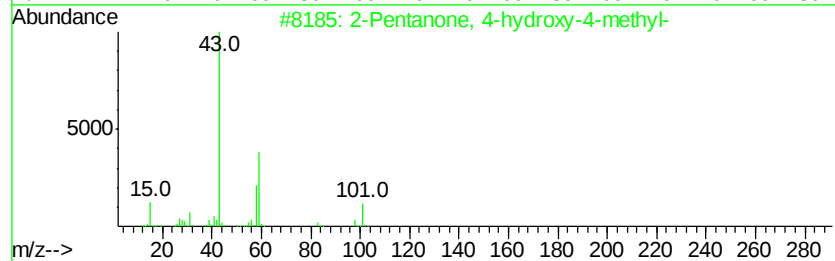
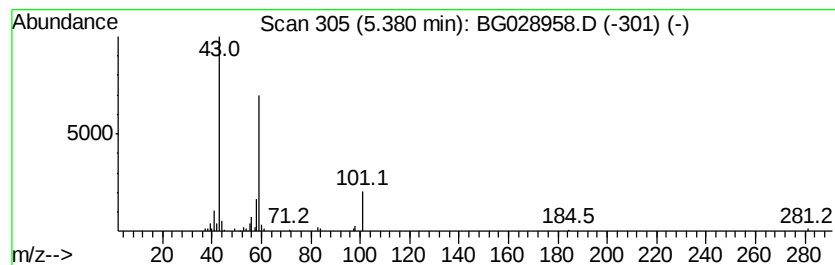
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.38	6.06 ng	61317	1,4-Dichlorobenzene-d4	8.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	40
3			Dimethadione	129	C5H7NO3	000695-53-4	36
4			Butanedioic acid, diazo-, dimeth...	172	C6H8N2O4	055514-36-8	25
5			3-Hexanol	102	C6H14O	000623-37-0	25



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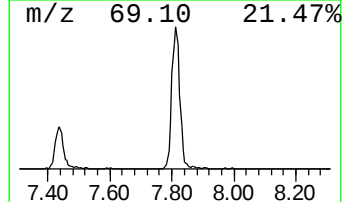
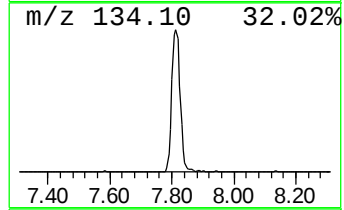
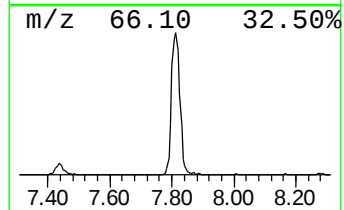
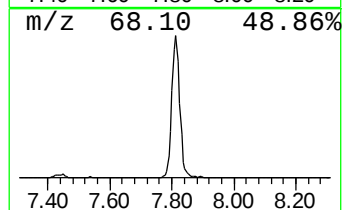
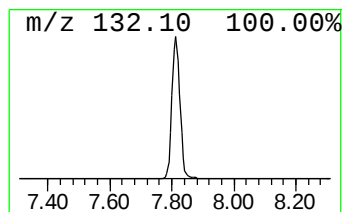
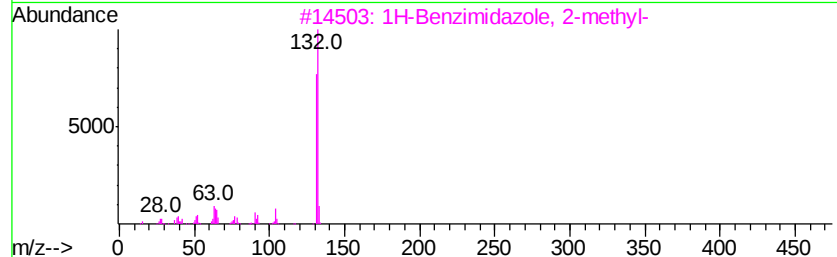
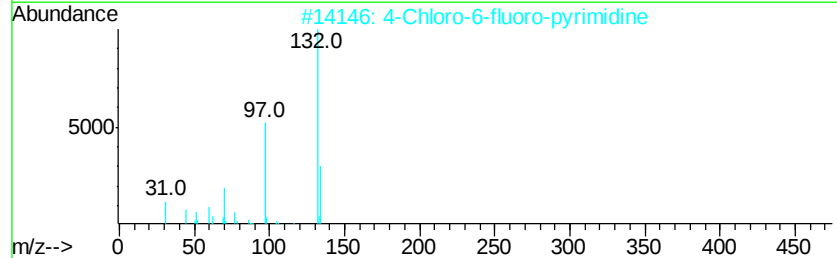
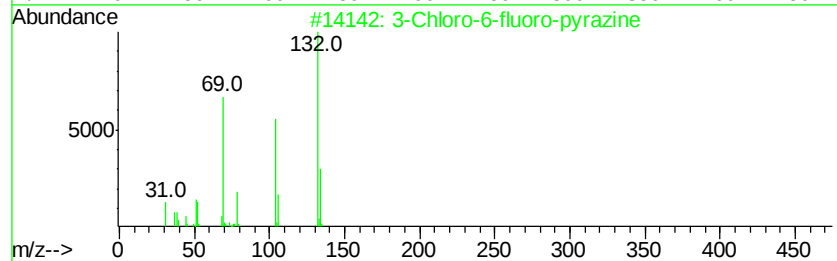
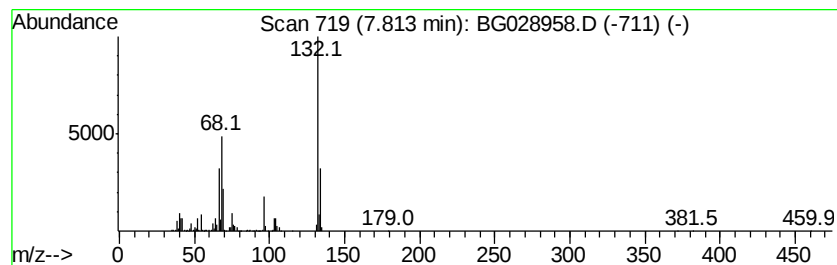
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Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	97.77 ng	989942	1,4-Dichlorobenzene-d4	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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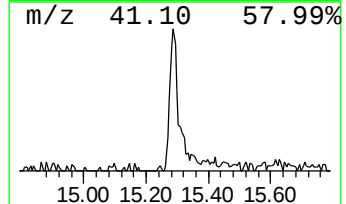
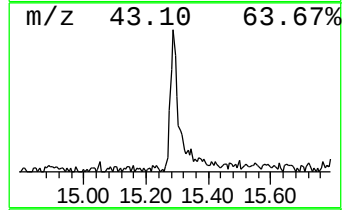
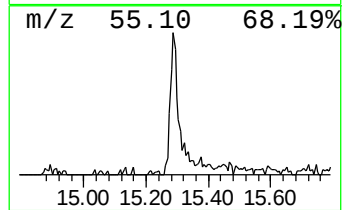
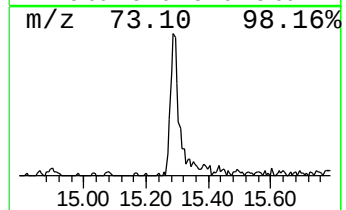
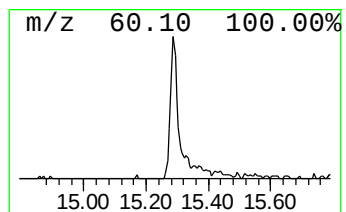
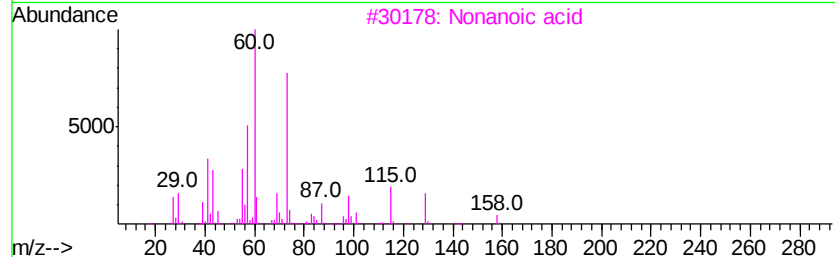
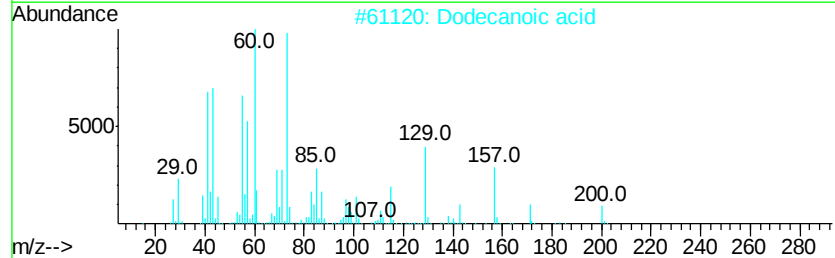
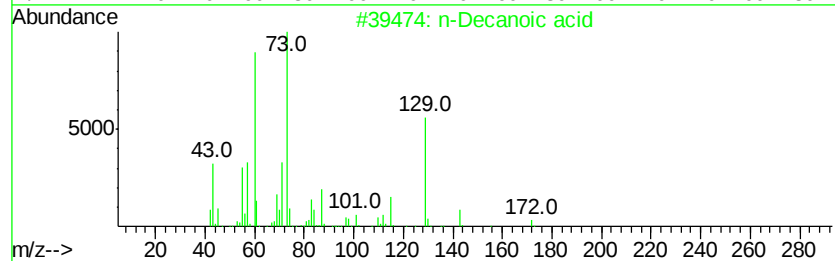
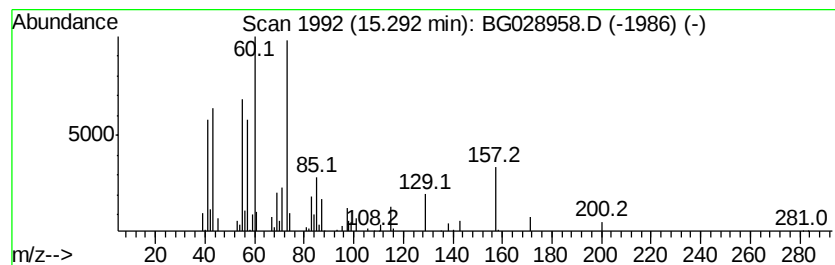
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Peak Number 4 n-Decanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	7.38 ng	169602	Acenaphthene-d10	14.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Decanoic acid	172 C10H20O2	000334-48-5	76
2	Dodecanoic acid	200 C12H24O2	000143-07-7	68
3	Nonanoic acid	158 C9H18O2	000112-05-0	47
4	Tetradecanoic acid	228 C14H28O2	000544-63-8	47
5	12-Bromododecanoic acid	278 C12H23BrO2	073367-80-3	22



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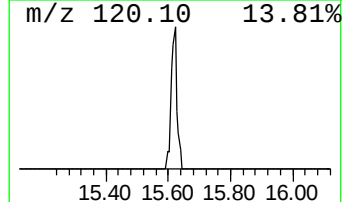
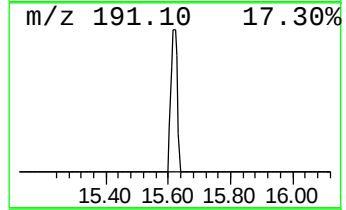
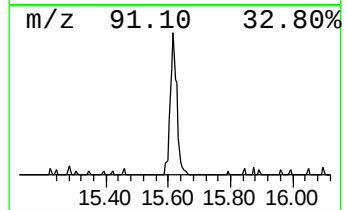
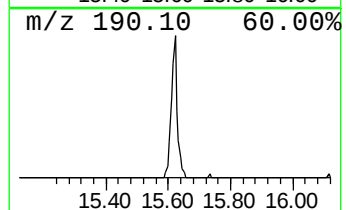
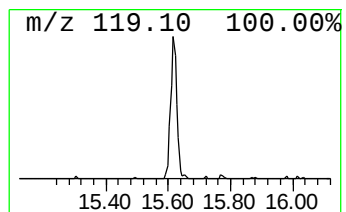
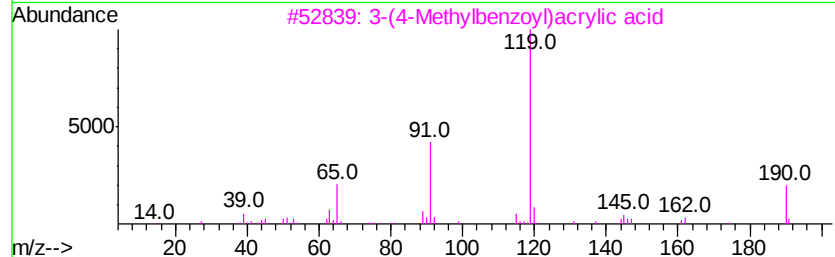
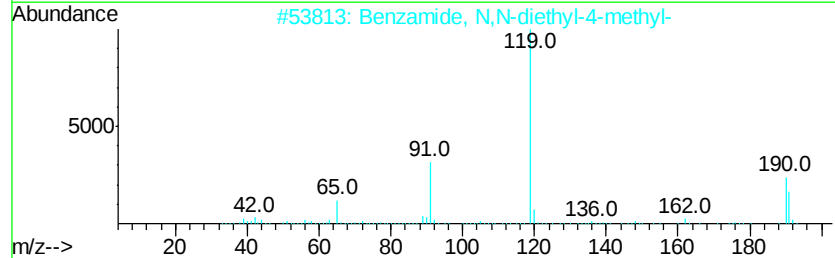
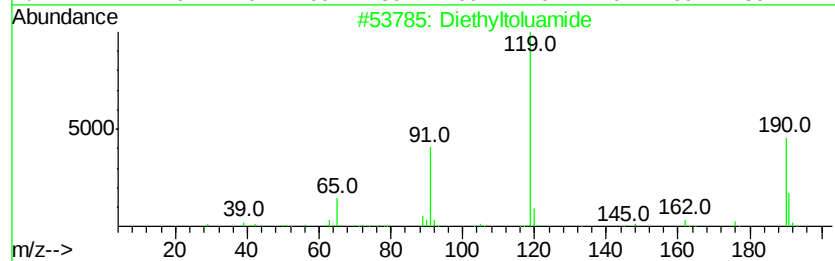
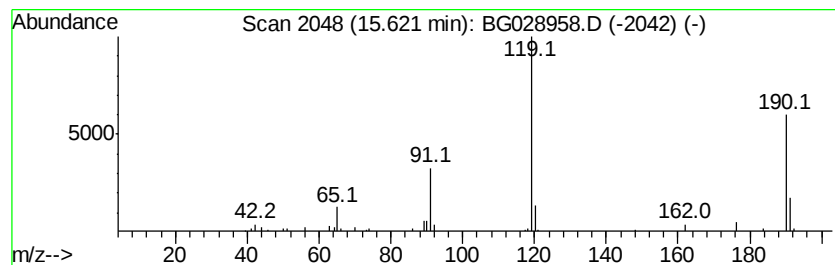
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Peak Number 5 Diethyltoluamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	2.66 ng	61179	Acenaphthene-d10	14.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Diethyltoluamide	191	C12H17NO	000134-62-3	96
2		Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	87
3		3-(4-Methylbenzoyl)acrylic acid	190	C11H10O3	020972-36-5	78
4		1-Propanone, 2-methyl-1-(4-methyl-...	162	C11H14O	050390-51-7	58
5		Benzamide, 3-methyl-N-[5-trifluo...	409	C18H14F7N02	339240-75-4	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.38	6.1	ng	61317	1	8.28	202495	20.0
unknown7.81	7.81	97.8	ng	989942	1	8.28	202495	20.0
n-Decanoic acid	15.29	7.4	ng	169602	3	14.89	459738	20.0
Diethyltoluamide	15.62	2.7	ng	61179	3	14.89	459738	20.0