

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092017\
 Data File : BG028832.D
 Acq On : 20 Sep 2017 15:16
 Operator : SJ/JU
 Sample : I5113-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RL-3-0-11.75-SPLPRE

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	5.395	300	307	315	rVB	55083	92864	1.41%	0.333%
2	5.859	379	386	398	rBV	640440	1073956	16.30%	3.855%
3	7.439	649	655	667	rBV	378784	695888	10.56%	2.498%
4	7.821	712	720	735	rBV	1106922	1934149	29.35%	6.944%
5	8.285	790	799	805	rBV2	113900	210009	3.19%	0.754%
6	8.615	846	855	866	rVB	918457	1655736	25.12%	5.944%
7	9.461	990	999	1009	rBV	800246	1477078	22.41%	5.303%
8	10.465	1155	1170	1183	rBV2	195306	597415	9.06%	2.145%
9	11.106	1272	1279	1284	rBV	160769	311804	4.73%	1.119%
10	11.159	1284	1288	1295	rVB	125462	220378	3.34%	0.791%
11	12.745	1552	1558	1569	rVB	80332	135819	2.06%	0.488%
12	12.962	1590	1595	1602	rVB	56634	99593	1.51%	0.358%
13	13.203	1626	1636	1648	rBV2	286116	617204	9.37%	2.216%
14	13.526	1684	1691	1699	rVB	2323808	3711575	56.32%	13.324%
15	14.907	1921	1926	1932	rVV2	286946	448509	6.81%	1.610%
16	14.972	1932	1937	1943	rVB	166523	266803	4.05%	0.958%
17	15.301	1983	1993	2001	rBV	99258	187344	2.84%	0.673%
18	15.953	2097	2104	2111	rVB2	151438	244861	3.72%	0.879%
19	16.400	2172	2180	2195	rBV	2268372	3745908	56.84%	13.448%
20	17.316	2328	2336	2343	rVB3	31375	67418	1.02%	0.242%
21	17.657	2388	2394	2398	rBV	420606	688129	10.44%	2.470%
22	17.698	2398	2401	2407	rVB	262871	409097	6.21%	1.469%
23	17.792	2414	2417	2423	rVB	45509	73681	1.12%	0.265%
24	18.062	2453	2463	2472	rBV	329008	561346	8.52%	2.015%
25	19.702	2736	2742	2748	rVB2	47885	84404	1.28%	0.303%
26	20.066	2799	2804	2813	rVB4	53833	97127	1.47%	0.349%
27	20.254	2826	2836	2842	rBV	4860565	6590431	100.00%	23.659%
28	21.981	3123	3130	3138	rBV2	441426	806562	12.24%	2.896%
29	25.454	3711	3721	3734	rVB	241542	750260	11.38%	2.693%

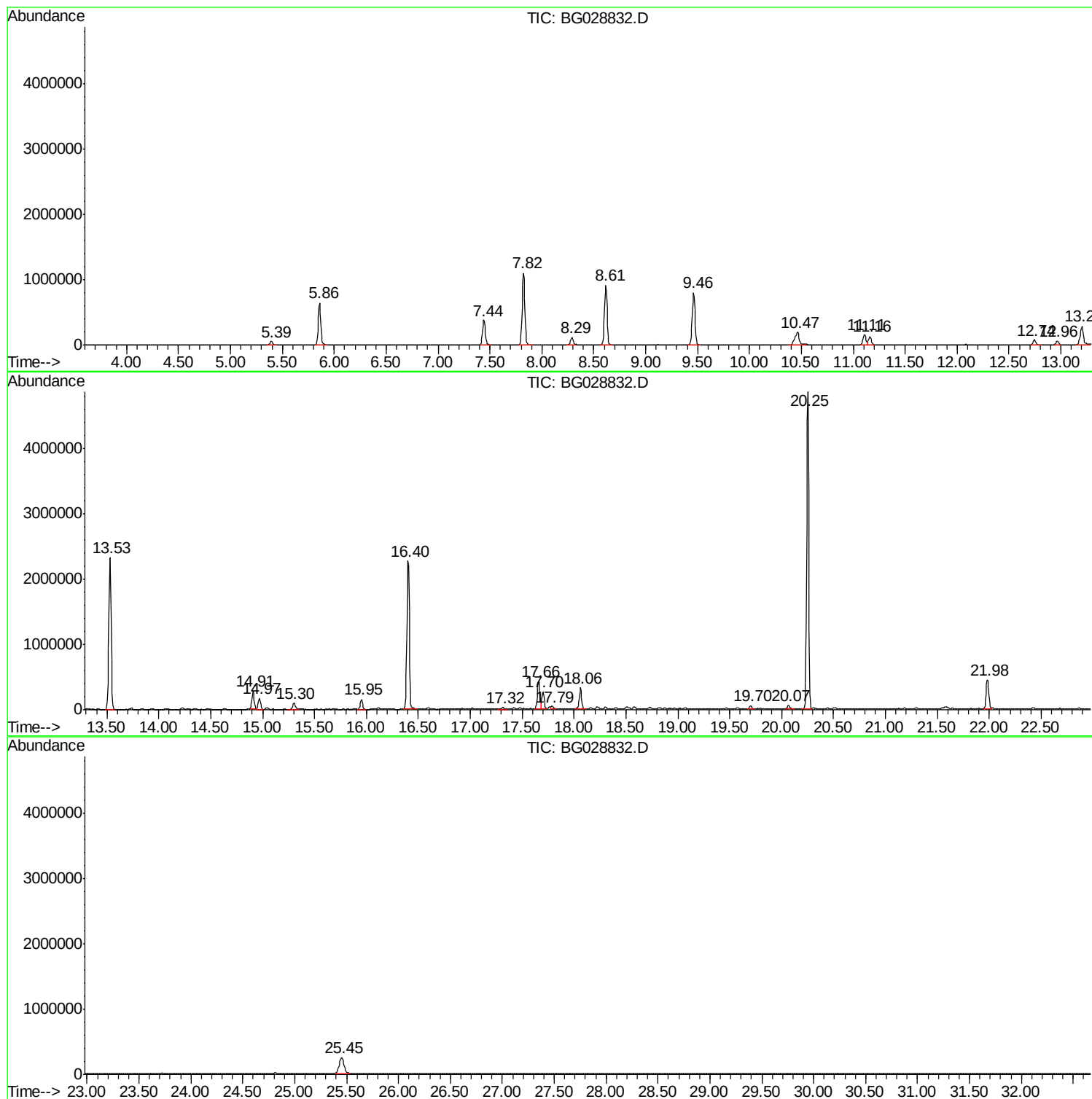
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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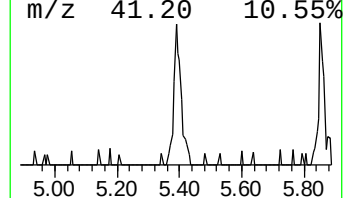
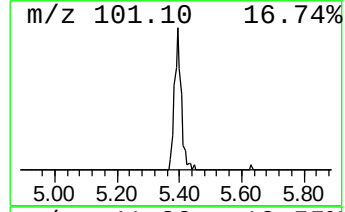
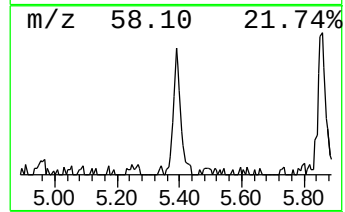
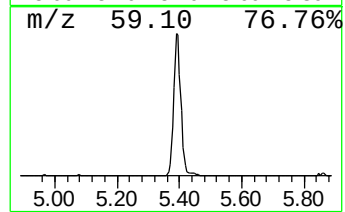
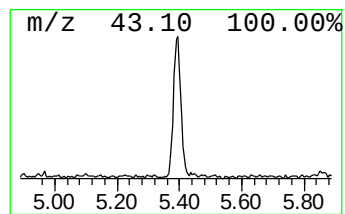
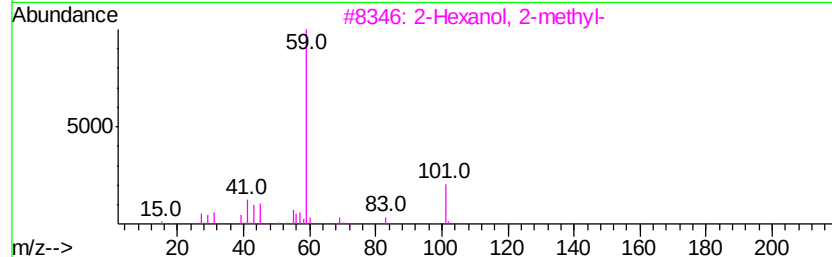
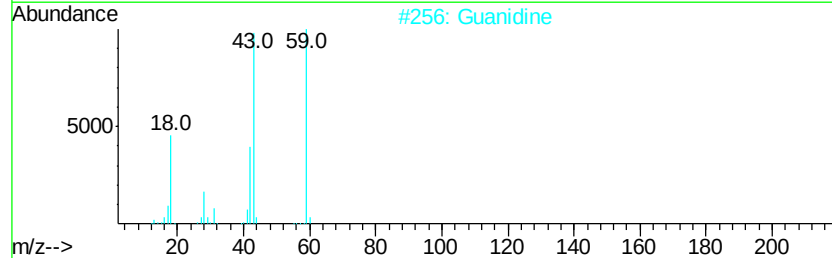
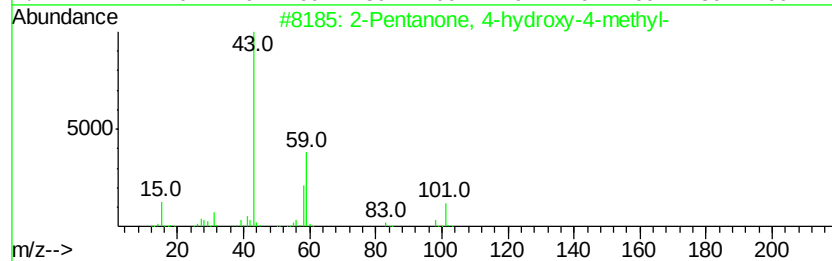
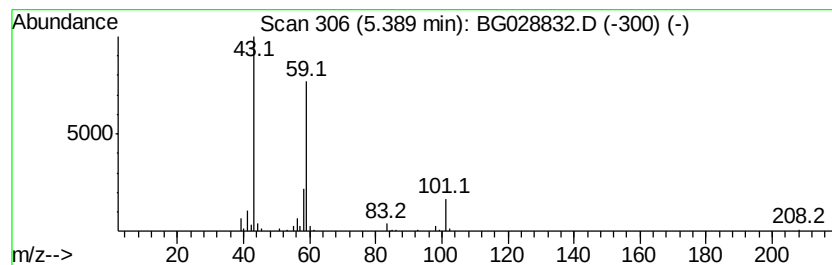
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
5.39	8.84 ng	92864	1,4-Dichlorobenzene-d4	8.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Guanidine	59	CH5N3	000113-00-8	50
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	36
4	3-Pentanol	88	C5H12O	000584-02-1	33
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	33



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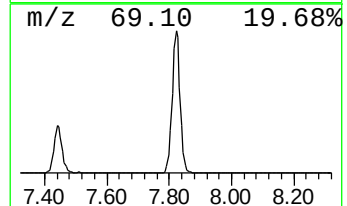
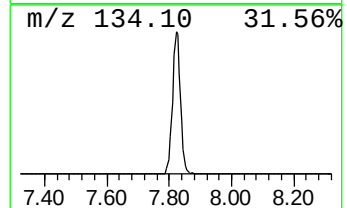
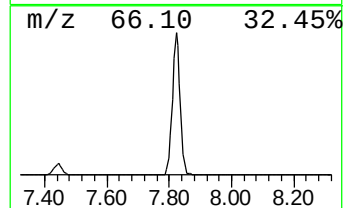
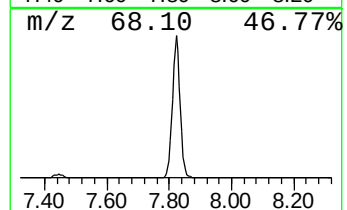
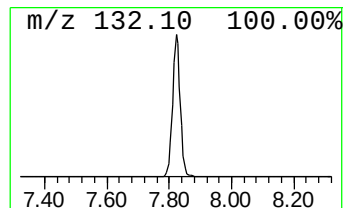
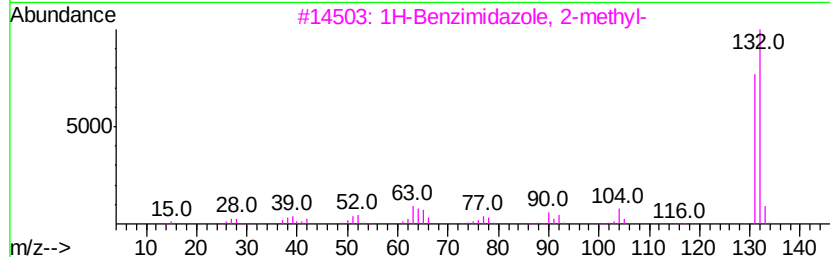
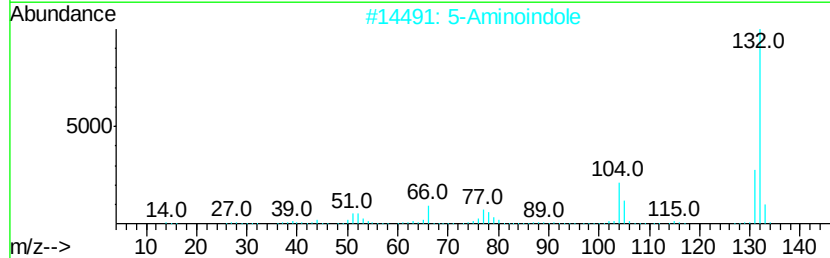
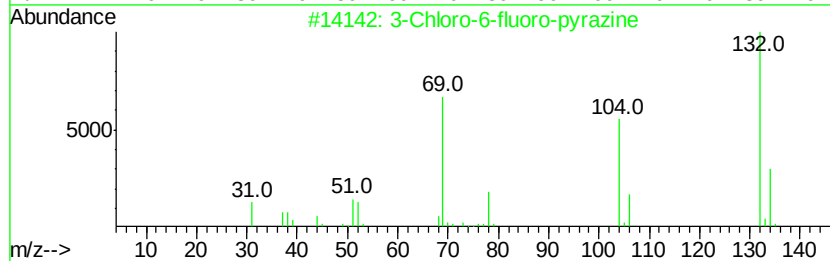
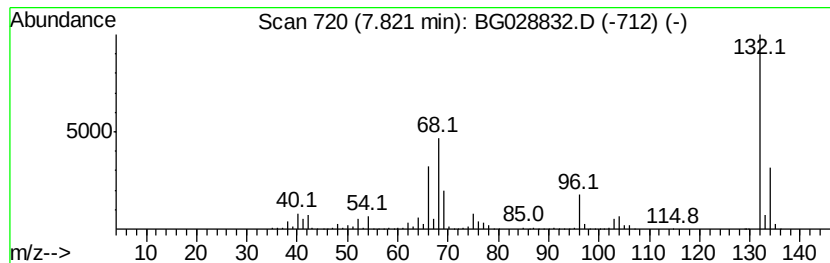
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Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	184.20 ng	1934150	1,4-Dichlorobenzene-d4	8.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	22
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5		N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10



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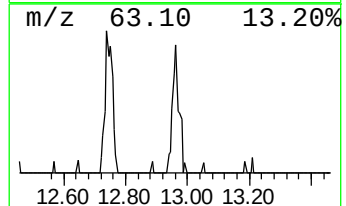
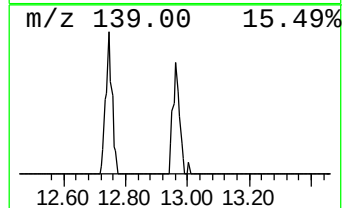
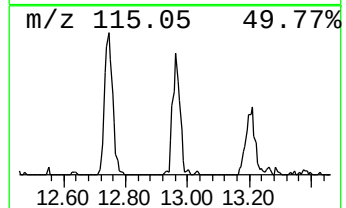
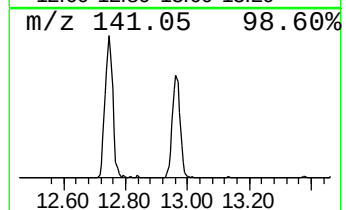
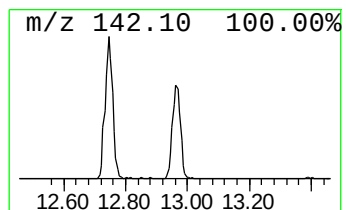
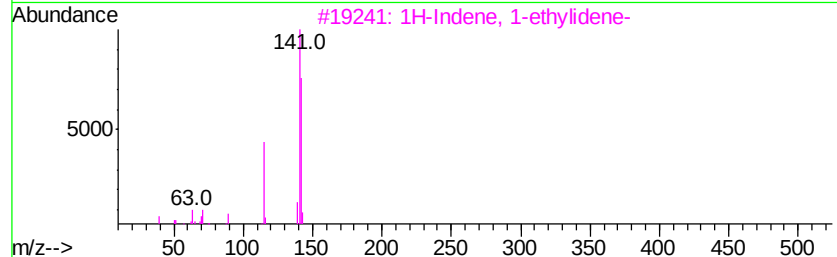
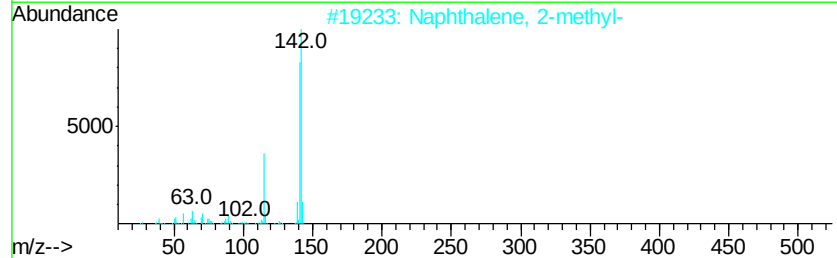
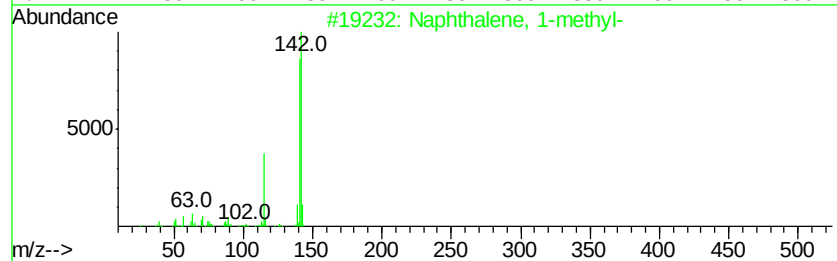
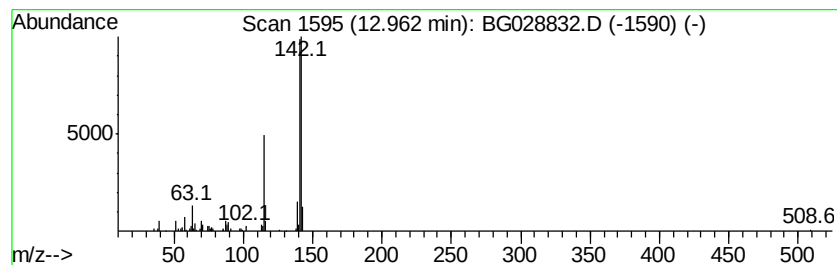
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Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	6.39 ng	99593	Naphthalene-d8	11.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
3		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5		Benzocycloheptatriene	142	C11H10	000264-09-5	90



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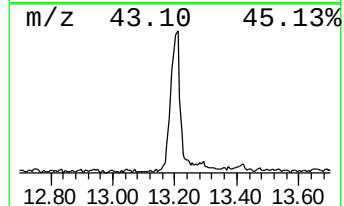
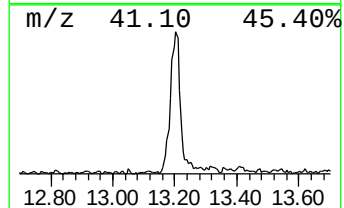
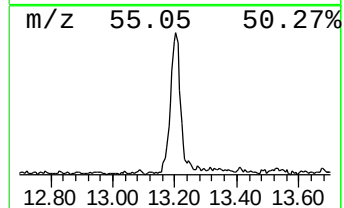
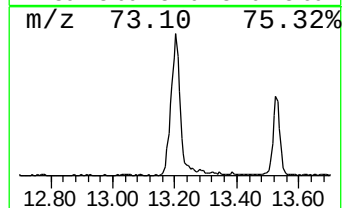
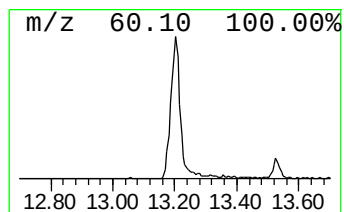
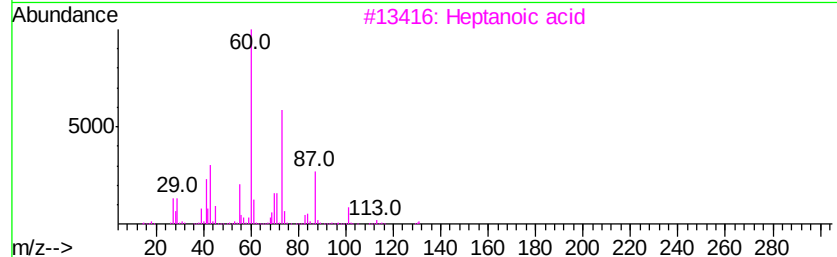
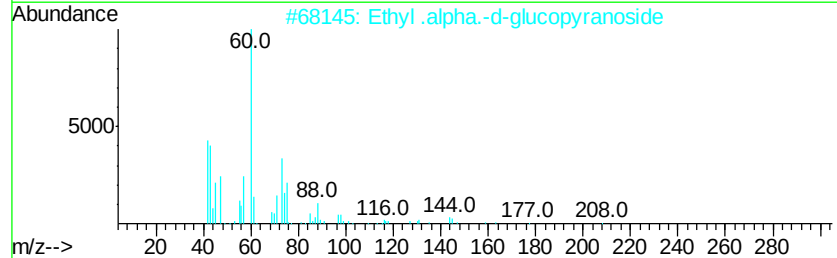
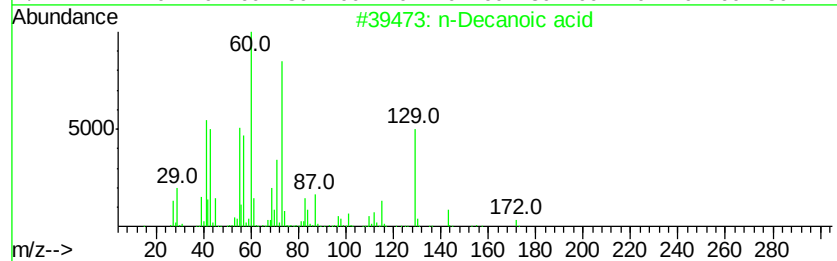
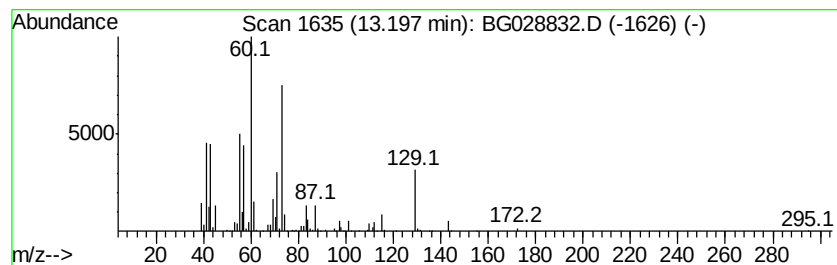
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Peak Number 5 n-Decanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	27.52 ng	617204	Acenaphthene-d10	14.91
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Decanoic acid	172 C10H20O2	000334-48-5 97
2		Ethyl .alpha.-d-glucopyranoside	208 C8H16O6	1000127-29-4 53
3		Heptanoic acid	130 C7H14O2	000111-14-8 50
4		Pentanoic acid	102 C5H10O2	000109-52-4 49
5		Butanoic acid, 3-methyl-	102 C5H10O2	000503-74-2 43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.39	8.8	ng	92864	1	8.29	210009	20.0
unknown7.82	7.82	184.2	ng	1934150	1	8.29	210009	20.0
Naphthalene, 1-me...	12.96	6.4	ng	99593	2	11.11	311804	20.0
n-Decanoic acid	13.20	27.5	ng	617204	3	14.91	448509	20.0