

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032718\
 Data File : BG033365.D
 Acq On : 27 Mar 2018 17:05
 Operator : SJ/JU
 Sample : J2048-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-108(12-13)

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-BG031918.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	3.483	26	33	43	rBV2	59813	127561	3.06%	0.630%
2	3.571	43	48	55	rVB	34266	56361	1.35%	0.279%
3	5.780	418	424	432	rVB	36930	66970	1.61%	0.331%
4	6.285	504	510	528	rBV	705880	1408748	33.80%	6.962%
5	7.972	790	797	816	rBV	751996	1635270	39.23%	8.081%
6	8.377	859	866	885	rBV	714845	1483436	35.59%	7.331%
7	8.871	941	950	966	rBV	94241	240784	5.78%	1.190%
8	9.200	997	1006	1025	rBV	535782	1123209	26.95%	5.551%
9	10.069	1146	1154	1176	rBV	403099	993708	23.84%	4.911%
10	11.750	1432	1440	1457	rBV	151231	339500	8.14%	1.678%
11	14.111	1835	1842	1859	rBV	1437128	2462915	59.09%	12.171%
12	14.905	1971	1977	1983	rBV	131531	214658	5.15%	1.061%
13	15.480	2069	2075	2088	rBV2	304977	547143	13.13%	2.704%
14	16.955	2319	2326	2345	rBV	1367857	2363232	56.69%	11.679%
15	17.102	2347	2351	2360	rVB	28128	51577	1.24%	0.255%
16	18.213	2530	2540	2554	rBV	445086	796431	19.11%	3.936%
17	19.012	2671	2676	2687	rBV3	58422	119091	2.86%	0.589%
18	20.733	2963	2969	2983	rBV	3053845	4168342	100.00%	20.599%
19	22.073	3193	3197	3208	rBV2	103026	205615	4.93%	1.016%
20	22.555	3272	3279	3288	rBV2	450134	917927	22.02%	4.536%
21	26.327	3910	3921	3942	rVB3	259811	913148	21.91%	4.513%

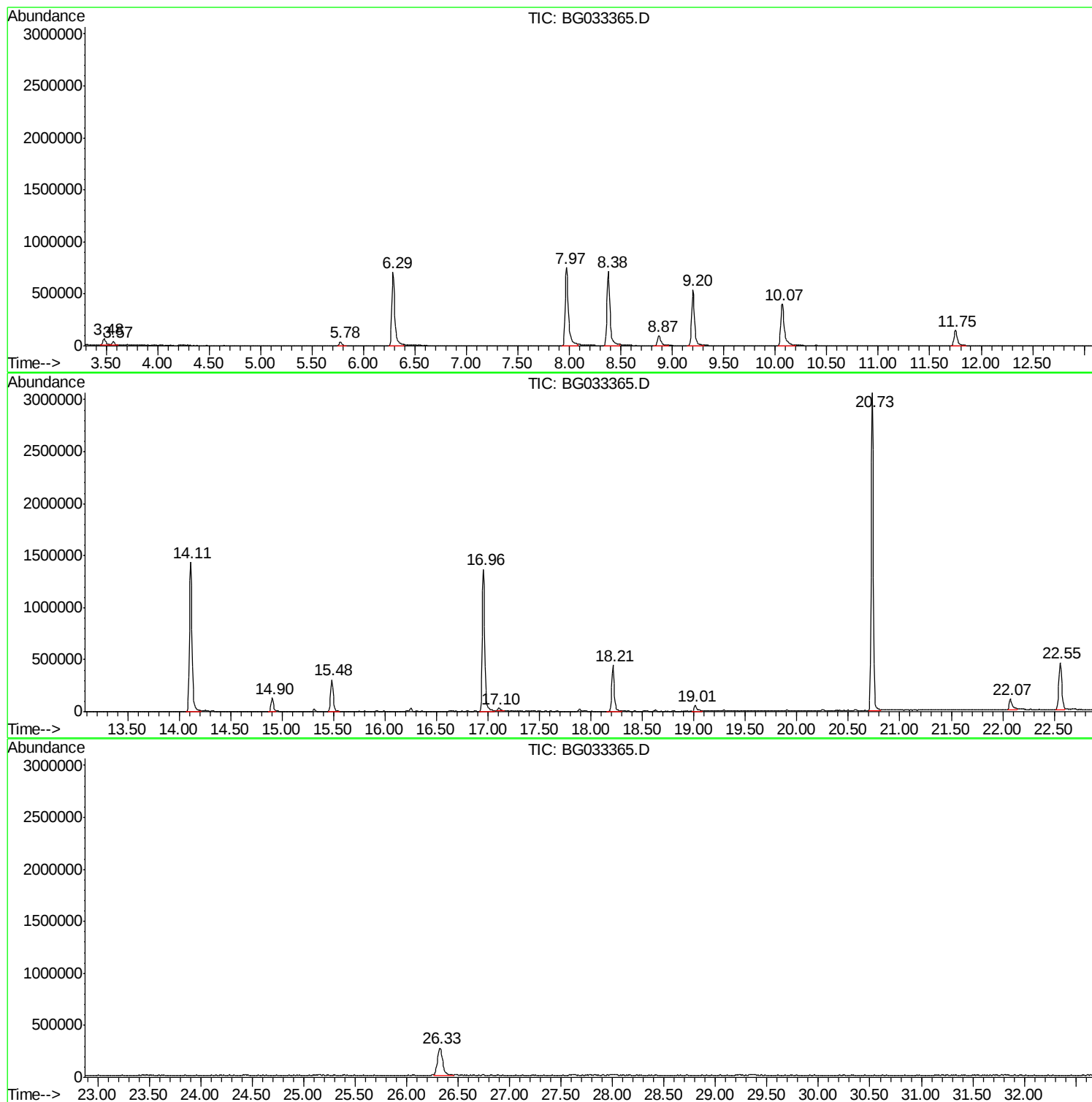
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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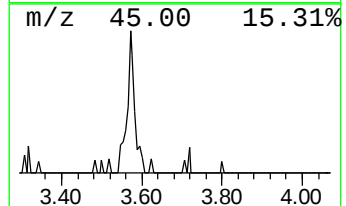
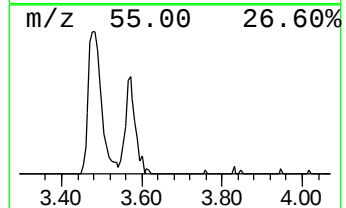
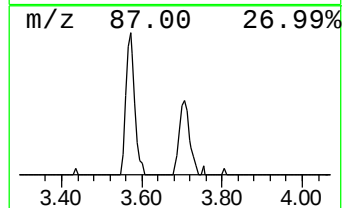
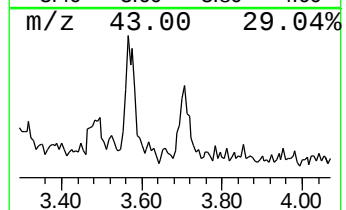
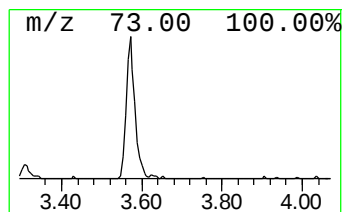
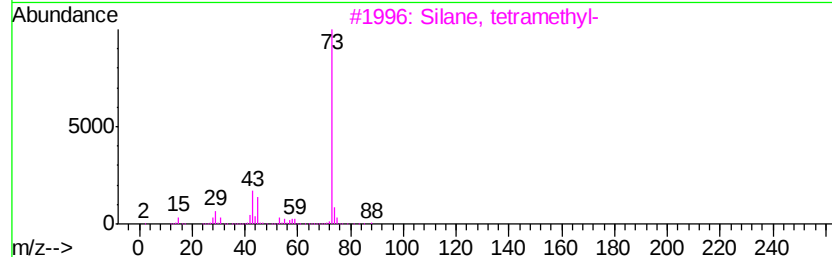
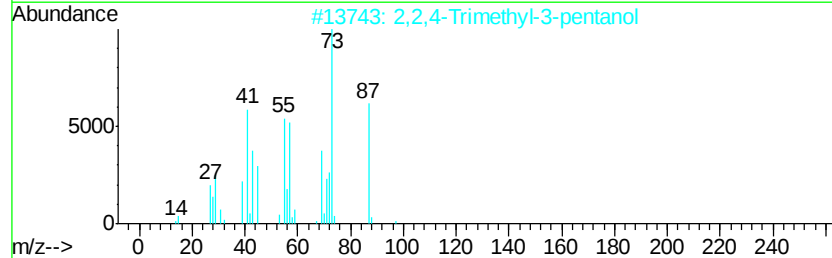
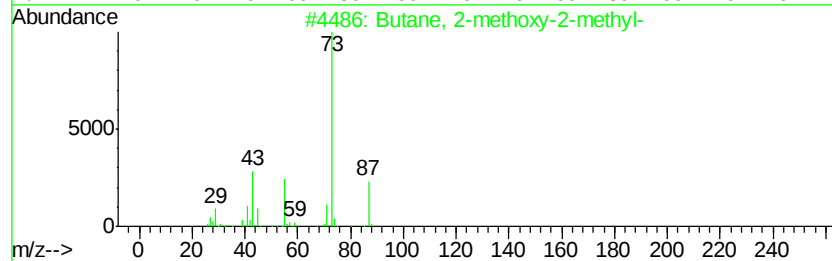
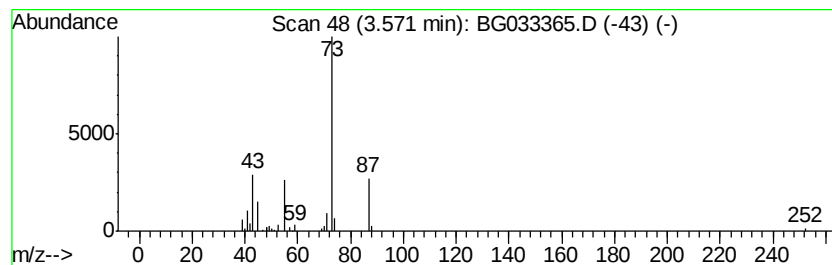
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	4.68 ng	56361	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	42
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10



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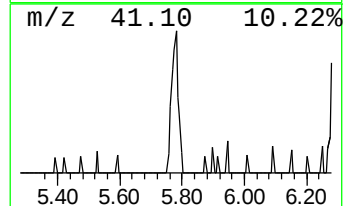
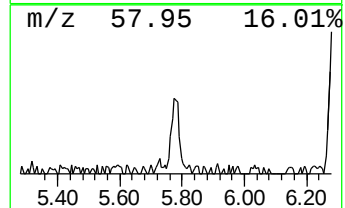
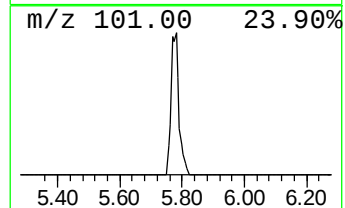
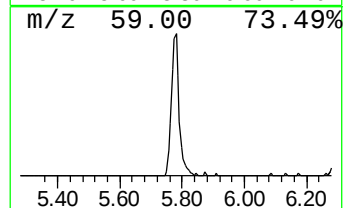
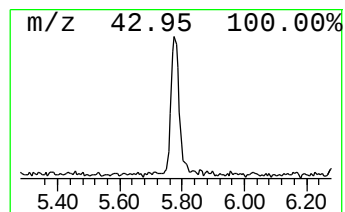
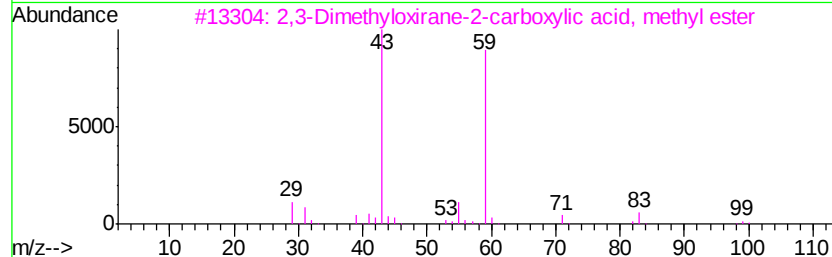
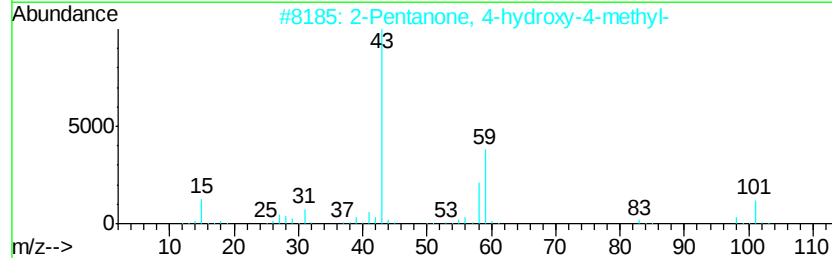
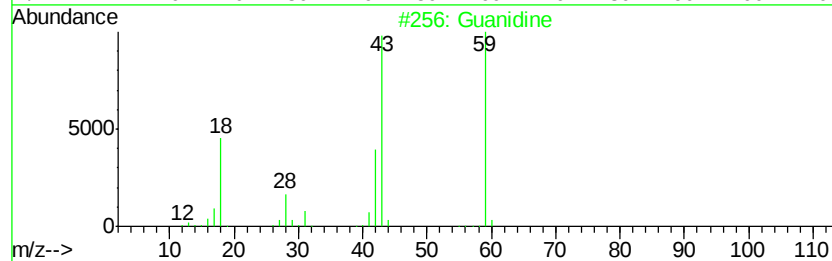
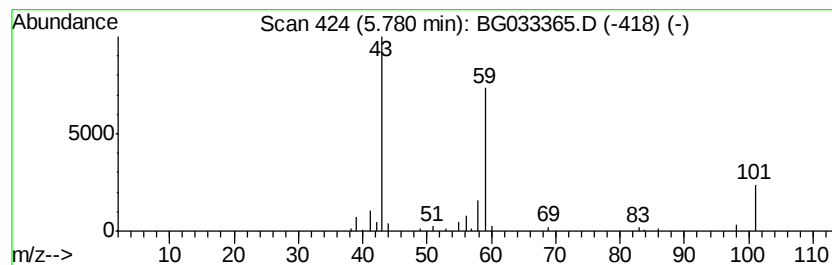
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Peak Number 3 Guanine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	5.56 ng	66970	1,4-Dichlorobenzene-d4	8.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanine		59	CH5N3	000113-00-8	50
2	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	38
3	2,3-Dimethyloxirane-2-carboxylic...		130	C6H10O3	1000306-64-4	36
4	3-Hexanol		102	C6H14O	000623-37-0	33
5	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33



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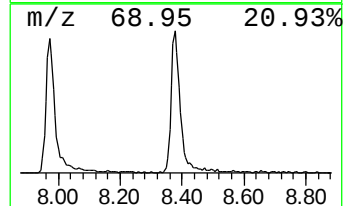
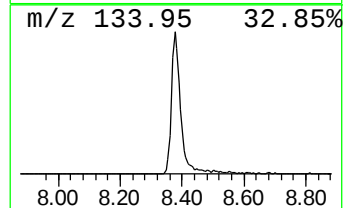
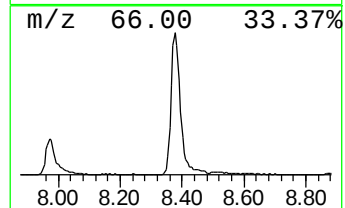
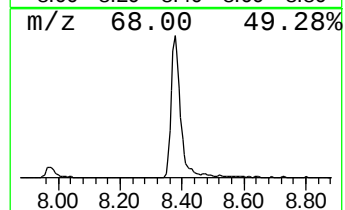
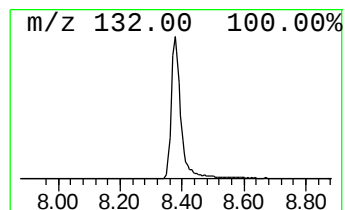
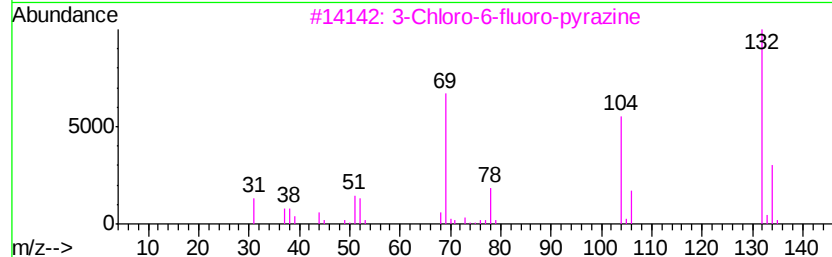
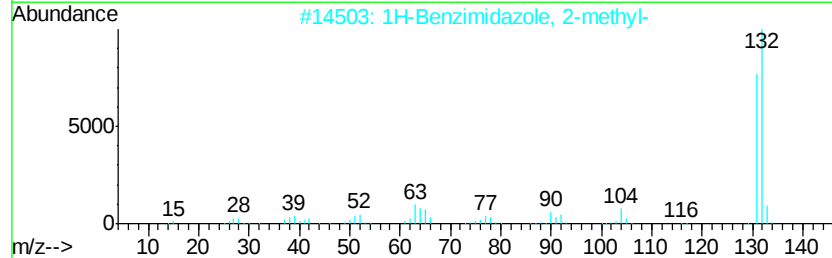
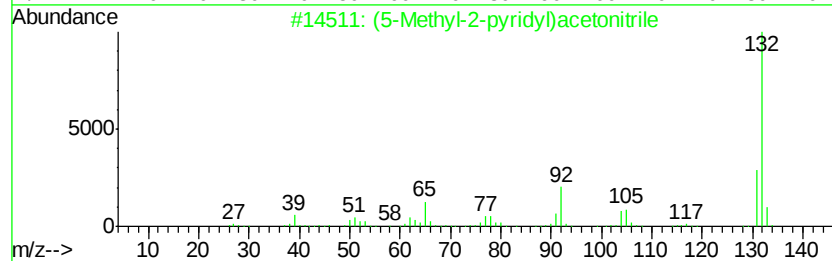
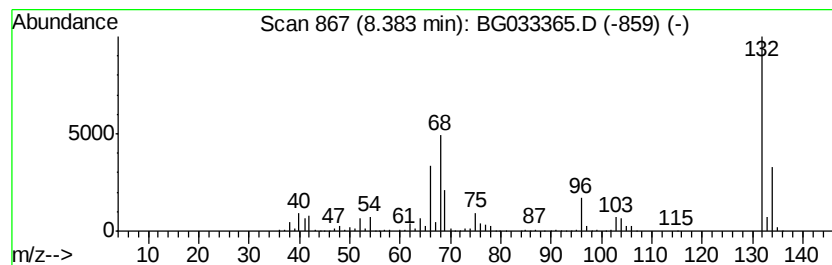
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Peak Number 4 unknown8.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	123.22 ng	1483440	1,4-Dichlorobenzene-d4	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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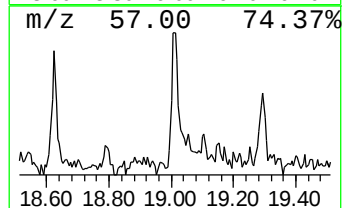
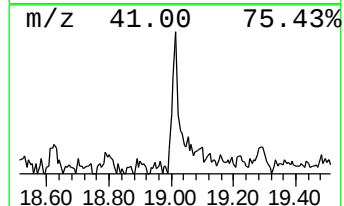
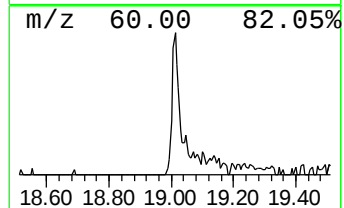
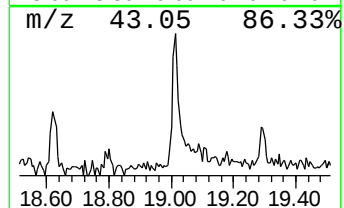
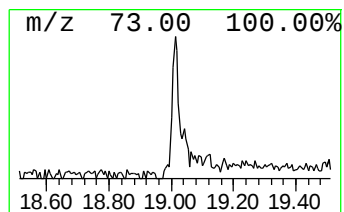
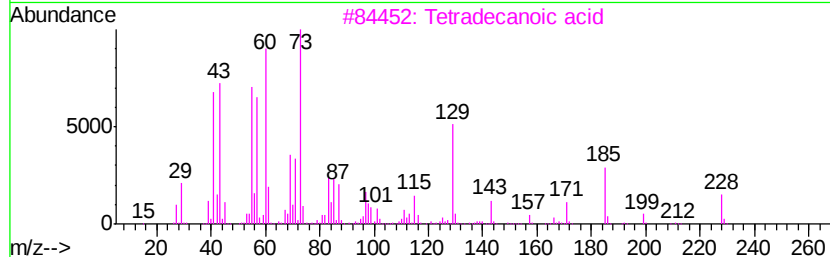
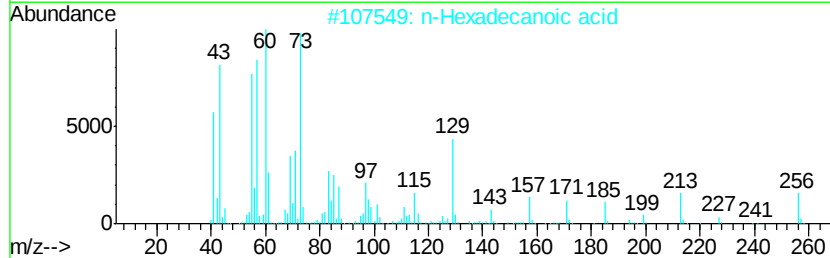
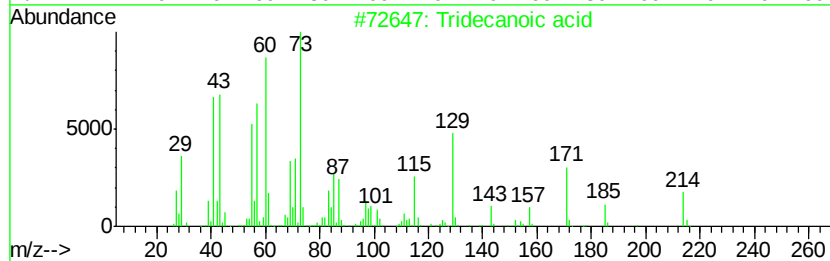
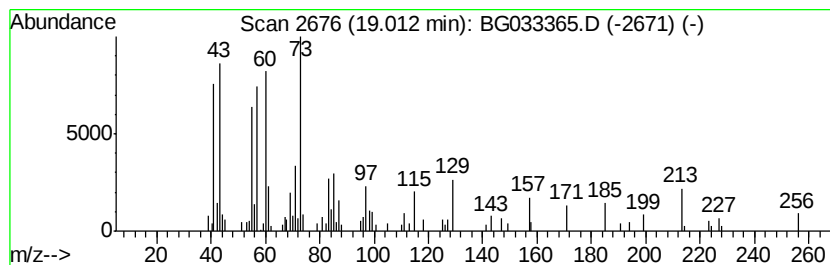
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Peak Number 6 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.01	2.99 ng	119091	Phenanthrene-d10		18.21
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	92
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52



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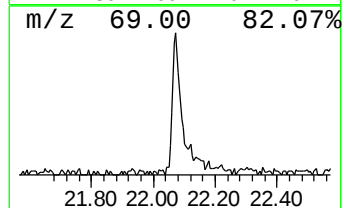
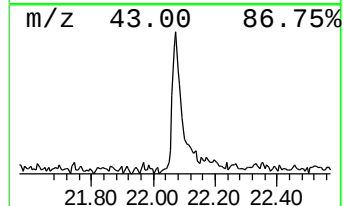
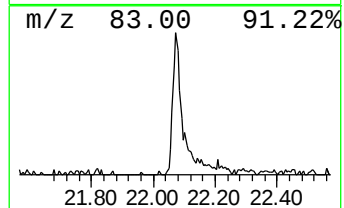
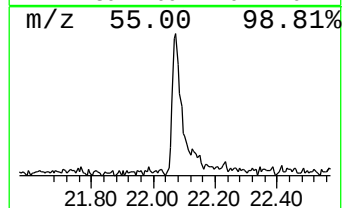
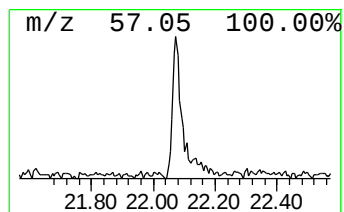
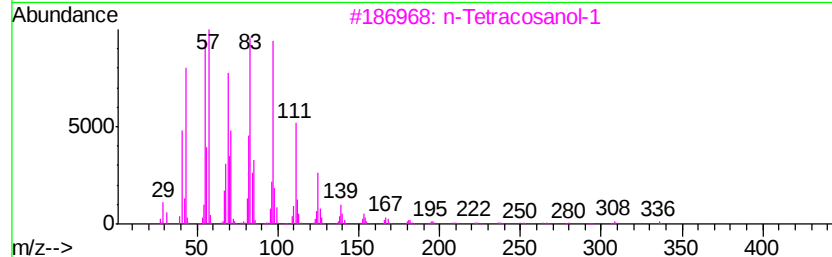
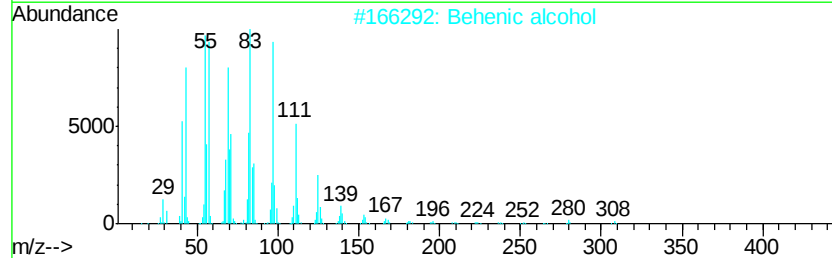
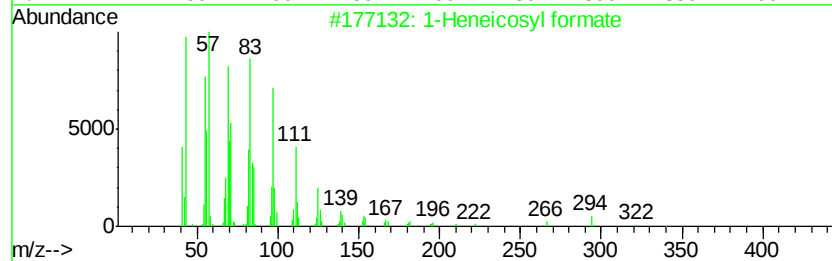
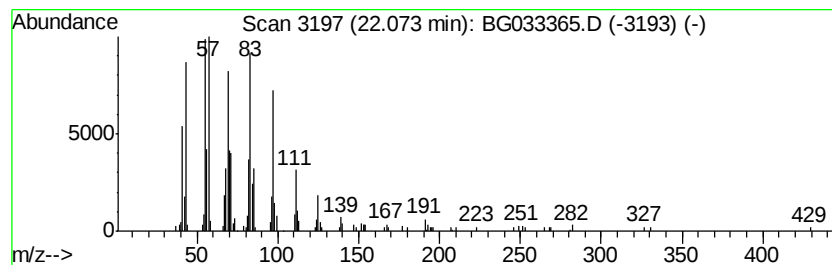
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Peak Number 7 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
22.07	4.48 ng	205615	Chrysene-d12		22.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl	formate	340	C22H44O2	077899-03-7	94
2	Behenic	alcohol	326	C22H46O	000661-19-8	94
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
4	n-Nonadecanol-1		284	C19H40O	001454-84-8	91
5	1-Heneicosanol		312	C21H44O	015594-90-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	4.7	ng	56361	1	8.87	240784	20.0
Guanidine	5.78	5.6	ng	66970	1	8.87	240784	20.0
unknown8.38	8.38	123.2	ng	1483440	1	8.87	240784	20.0
Tridecanoic acid	19.01	3.0	ng	119091	4	18.21	796431	20.0
1-Heneicosyl formate	22.07	4.5	ng	205615	5	22.56	917927	20.0