

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082120\
 Data File : BM027190.D
 Acq On : 22 Aug 2020 03:31
 Operator : JU/CG
 Sample : L3719-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 20200511-AMENDED-DISCRETE-00

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082120.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	4.781	299	305	315	rBV	1480371	1927181	54.93%	7.573%
2	5.234	376	382	392	rBV	710759	990652	28.23%	3.893%
3	6.798	639	648	661	rVB	1417015	2221024	63.30%	8.727%
4	6.910	661	667	675	rVB	52856	88793	2.53%	0.349%
5	7.228	715	721	731	rBV2	22245	42198	1.20%	0.166%
6	7.610	780	786	793	rBV	553562	850561	24.24%	3.342%
7	8.751	973	980	992	rBV	1036890	1684889	48.02%	6.621%
8	9.098	1032	1039	1046	rBV	126870	208778	5.95%	0.820%
9	10.381	1248	1257	1265	rBV	659940	1072066	30.56%	4.213%
10	10.722	1310	1315	1323	rBV2	16510	42620	1.21%	0.167%
11	12.869	1673	1680	1686	rBV	2064022	2923596	83.33%	11.488%
12	12.969	1691	1697	1702	rVB	31532	50952	1.45%	0.200%
13	13.710	1815	1823	1830	rBV	233317	319249	9.10%	1.254%
14	14.251	1908	1915	1922	rBV	911455	1367828	38.98%	5.375%
15	15.739	2162	2168	2178	rBV	531326	729510	20.79%	2.867%
16	15.951	2195	2204	2210	rBV	68970	108744	3.10%	0.427%
17	16.392	2274	2279	2286	rBV2	42547	70973	2.02%	0.279%
18	16.745	2333	2339	2344	rBV2	47713	86855	2.48%	0.341%
19	16.992	2375	2381	2392	rVB	1166377	1601912	45.66%	6.295%
20	17.910	2533	2537	2547	rBV	154204	235617	6.72%	0.926%
21	19.057	2727	2732	2737	rBV	75485	115310	3.29%	0.453%
22	19.198	2752	2756	2762	rBV3	44300	69771	1.99%	0.274%
23	19.415	2790	2793	2801	rVB	64662	95711	2.73%	0.376%
24	19.633	2825	2830	2837	rBV	3083559	3508626	100.00%	13.787%
25	20.921	3045	3049	3057	rBV	403058	541538	15.43%	2.128%
26	21.127	3082	3084	3087	rBV	43311	46934	1.34%	0.184%
27	21.186	3089	3094	3099	rBV	1641132	2077862	59.22%	8.165%
28	22.750	3357	3360	3365	rVB2	148203	201236	5.74%	0.791%
29	23.374	3459	3466	3479	rVB	1147920	2167813	61.79%	8.518%

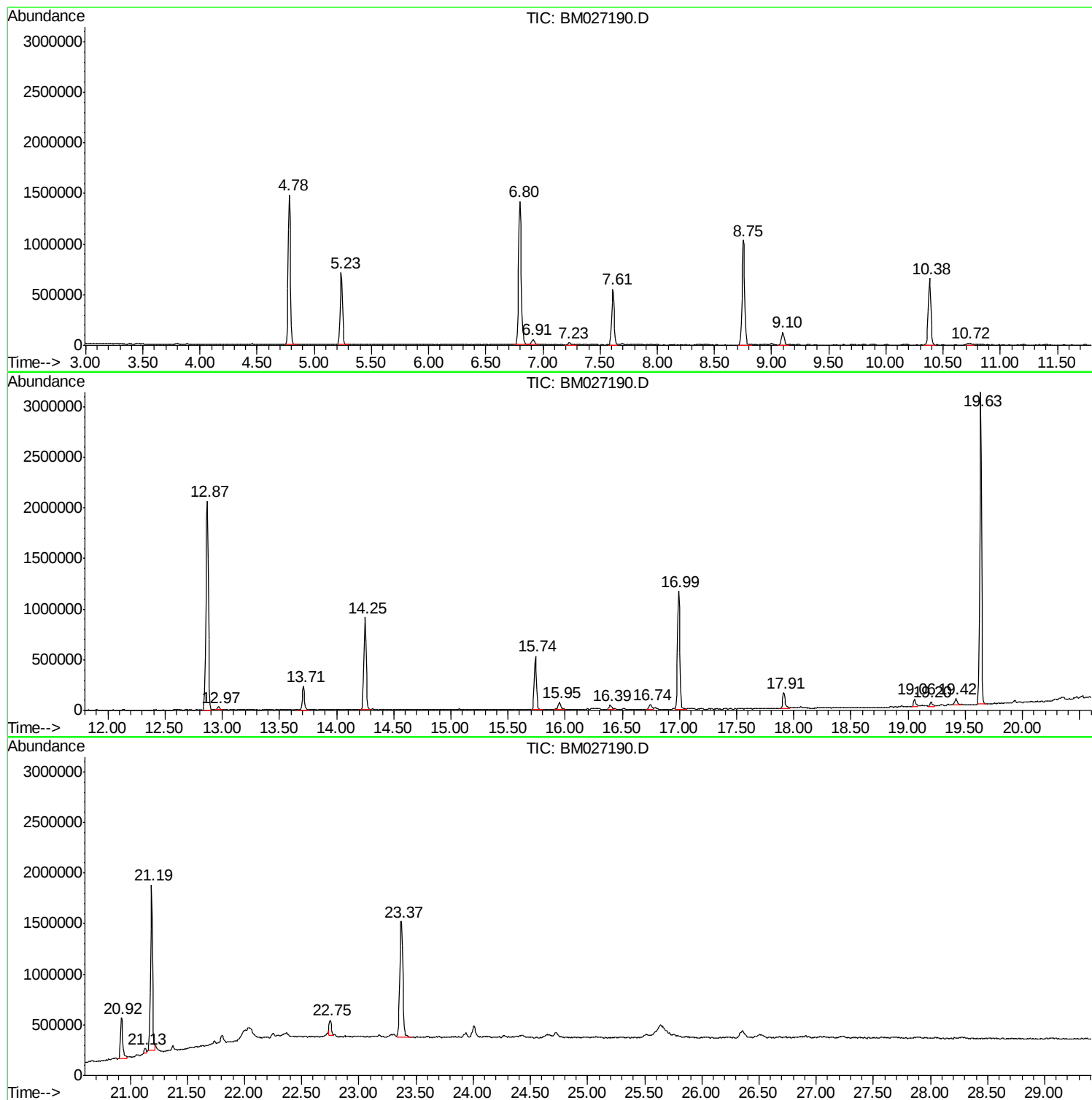
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082120.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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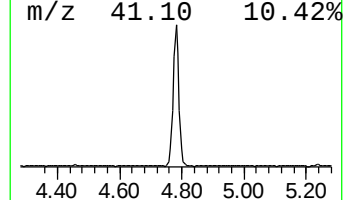
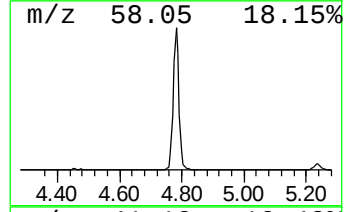
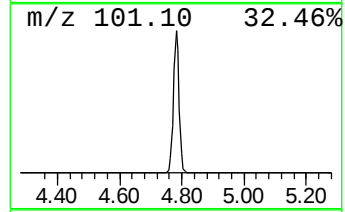
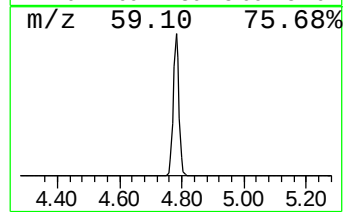
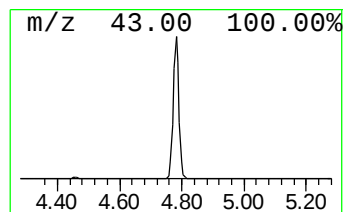
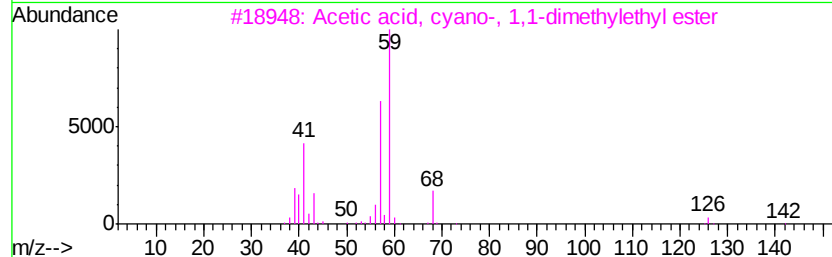
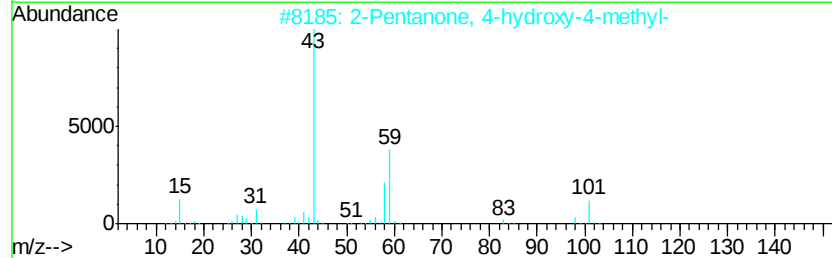
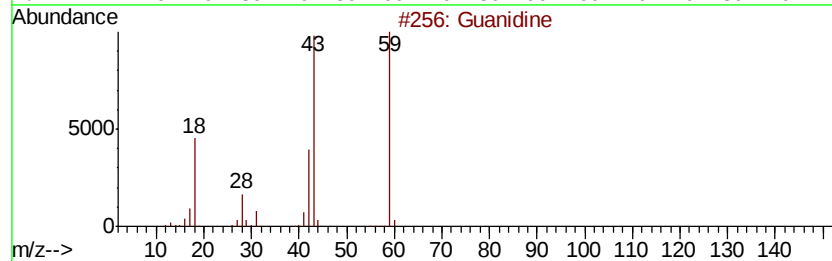
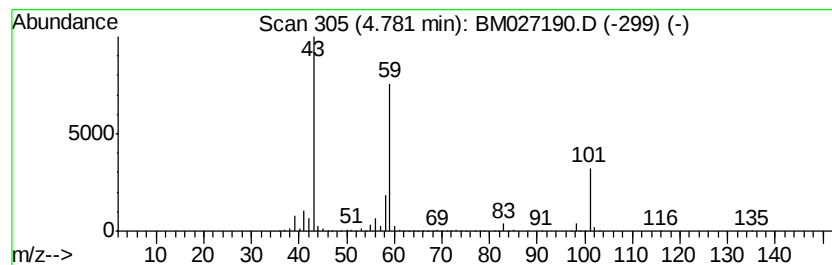
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Guanidine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	45.32 ng	1927180	1,4-Dichlorobenzene-d4	7.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Guanidine	59	CH5N3	000113-00-8	50
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	38
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	35
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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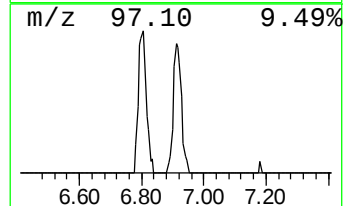
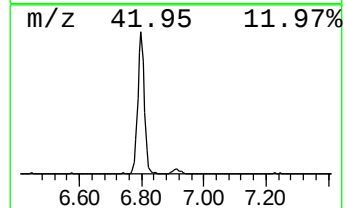
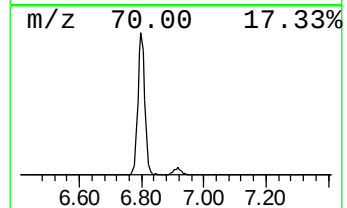
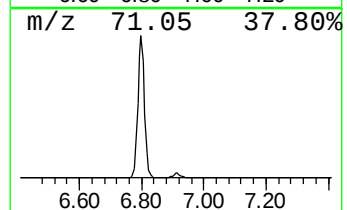
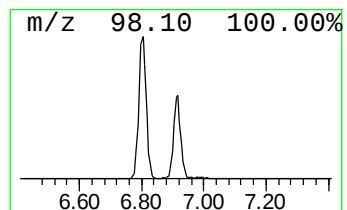
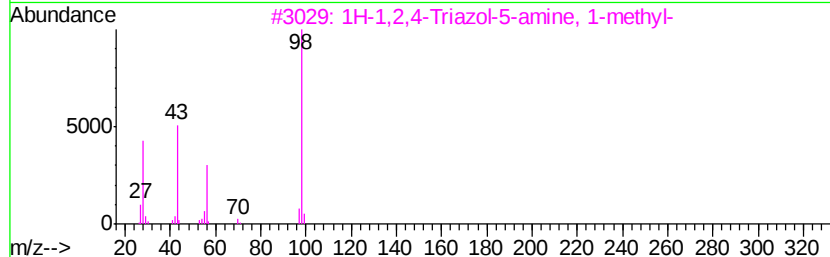
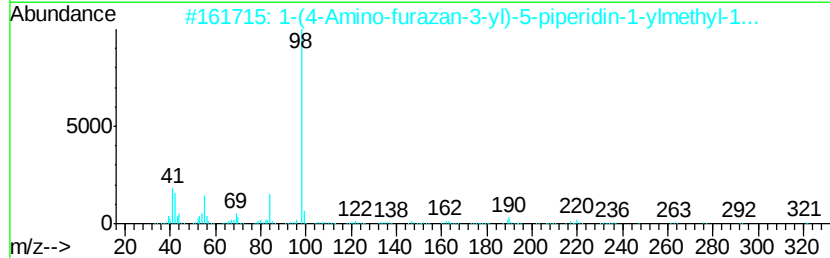
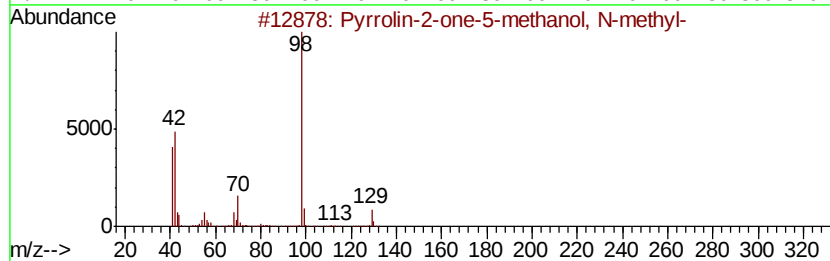
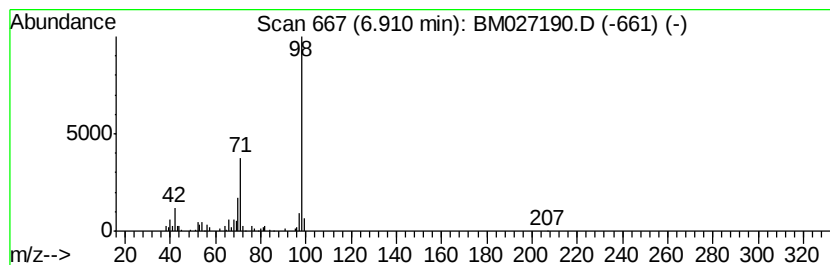
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Peak Number 2 Pyrrolin-2-one-5-methanol, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.91	2.09 ng	88793	1,4-Dichlorobenzene-d4	7.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrrolin-2-one-5-methanol, N-met...	129	C6H11N02	1000125-98-2	59
2		1-(4-Amino-furazan-3-yl)-5-piper...	321	C13H19N7O3	311314-85-9	53
3		1H-1,2,4-Triazol-5-amine, 1-methyl-	98	C3H6N4	015795-39-8	53
4		3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	50
5		1,3,4-Thiadiazole-2(3H)-thione, ...	229	C9H15N3S2	1000338-18-2	50



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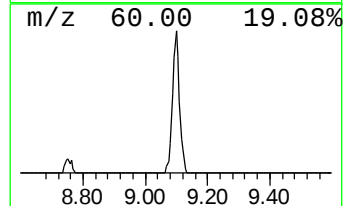
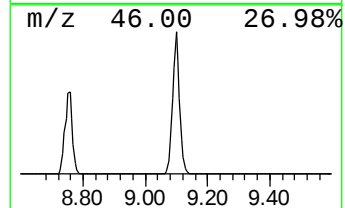
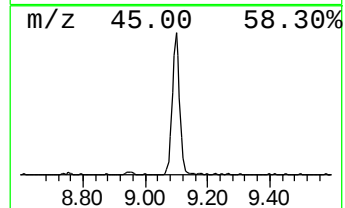
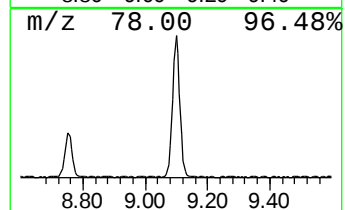
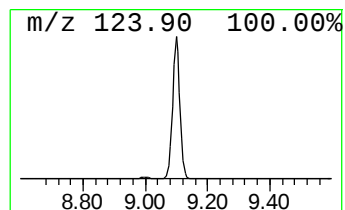
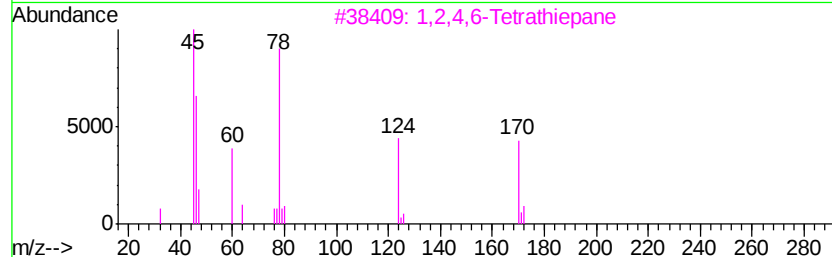
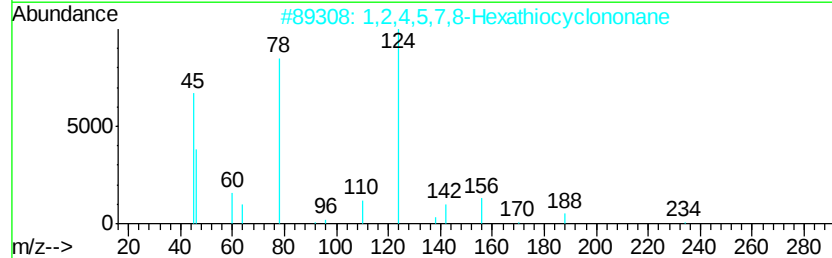
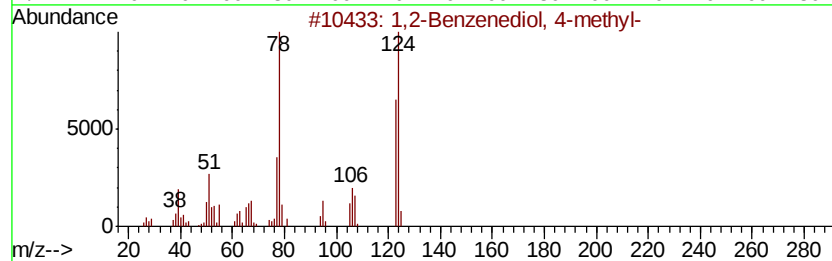
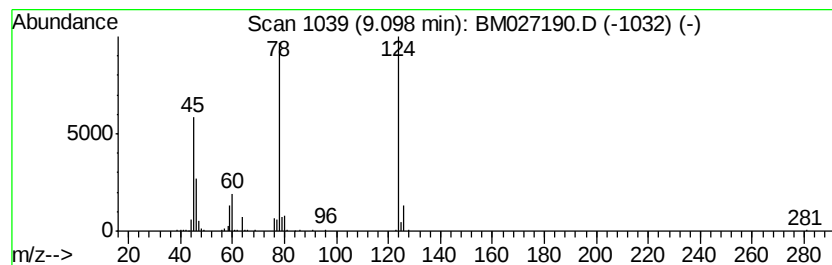
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Peak Number 3 unknown9.10 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.10	3.89 ng	208778	Naphthalene-d8	10.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	45
2		1,2,4,5,7,8-Hexathiocyclononane	234	C3H6S6	081531-38-6	43
3		1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	10
4		Propanedinitrile, methylene-	78	C4H2N2	000922-64-5	9
5		Fumaronitrile	78	C4H2N2	000764-42-1	9



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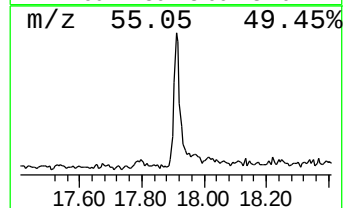
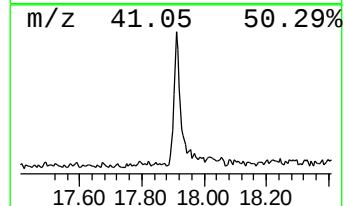
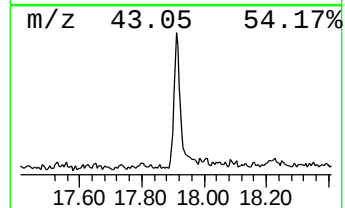
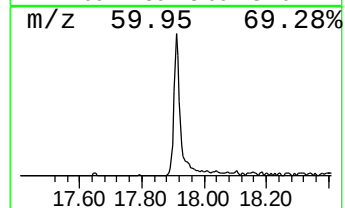
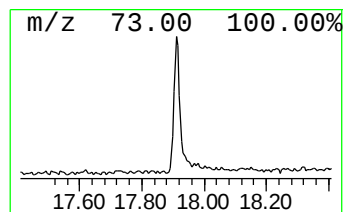
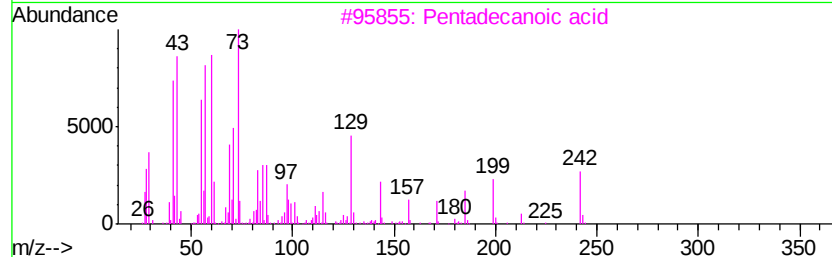
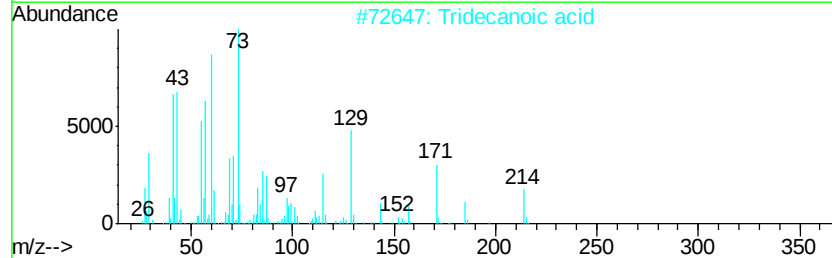
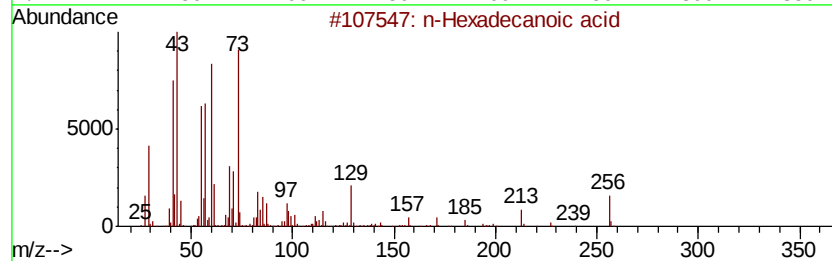
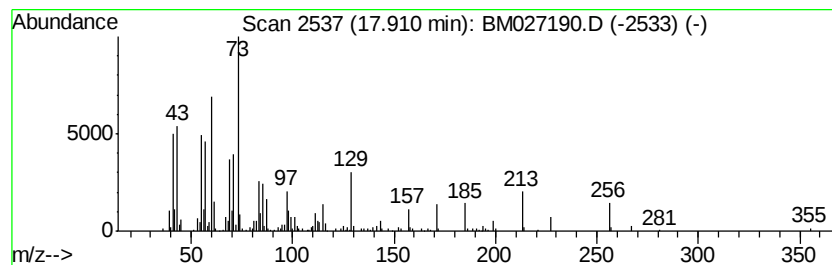
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.91	2.94 ng	235617	Phenanthrene-d10		16.99	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4		Octadecanoic acid	284	C18H36O2	000057-11-4	50
5		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50



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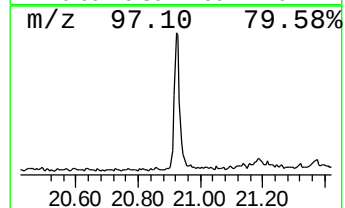
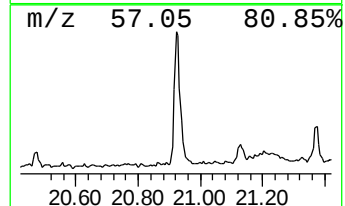
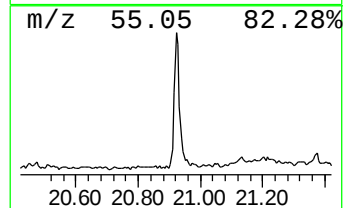
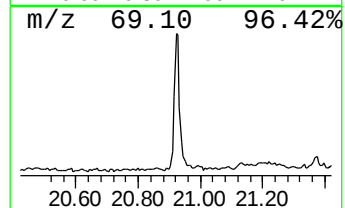
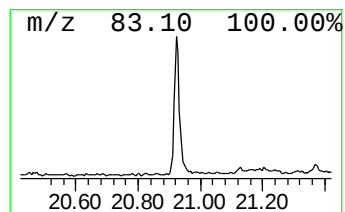
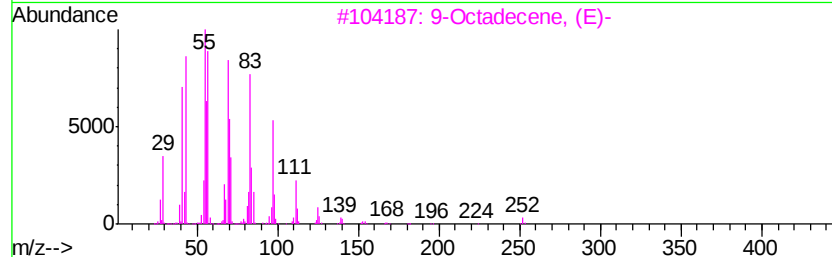
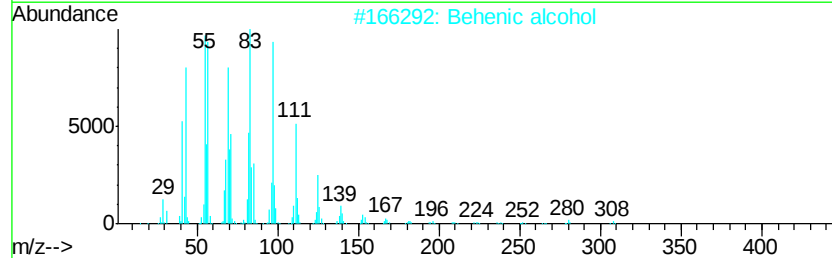
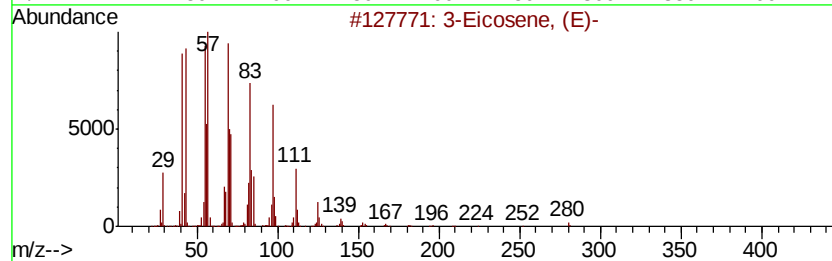
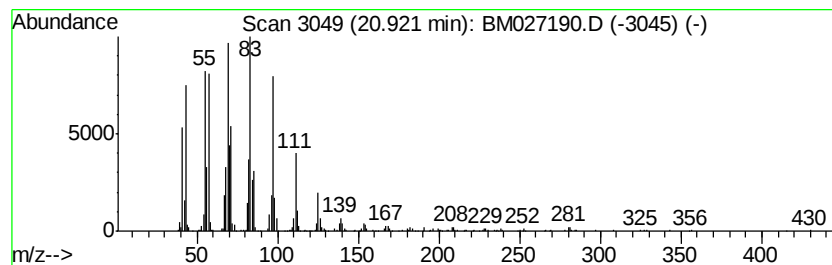
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Peak Number 5 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.92	5.21 ng	541538	Chrysene-d12	21.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2		Behenic alcohol	326	C22H46O	000661-19-8	89
3		9-Octadecene, (E)-	252	C18H36	007206-25-9	87
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83
5		Cyclotetradecane	196	C14H28	000295-17-0	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Guanidine	4.78	45.3	ng	1927180	1	7.61	850561	20.0
Pyrrolin-2-one-5-...	6.91	2.1	ng	88793	1	7.61	850561	20.0
unknown9.10	9.10	3.9	ng	208778	2	10.38	1072070	20.0
n-Hexadecanoic acid	17.91	2.9	ng	235617	4	16.99	1601910	20.0
3-Eicosene, (E)-	20.92	5.2	ng	541538	5	21.19	2077860	20.0