

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
 Data File : BG043476.D
 Acq On : 1 Nov 2019 21:49
 Operator : JU
 Sample : K5620-07 2X
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-26A-S

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_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	3.190	12	17	25	rVB	44866	86816	6.84%	0.857%
2	5.123	341	346	357	rBV	56727	95297	7.51%	0.941%
3	5.599	419	427	439	rBV	264545	489525	38.56%	4.835%
4	7.197	691	699	710	rBV	271099	541717	42.67%	5.350%
5	7.556	752	760	770	rBV	307208	563203	44.37%	5.562%
6	8.014	831	838	847	rBV	183359	325310	25.63%	3.213%
7	8.337	886	893	906	rBV2	244232	443651	34.95%	4.382%
8	9.178	1028	1036	1047	rBV2	145428	319606	25.18%	3.156%
9	10.817	1307	1315	1334	rBV	211020	441867	34.81%	4.364%
10	13.267	1722	1732	1745	rBV	474268	854240	67.29%	8.437%
11	14.089	1865	1872	1887	rBV	65110	121454	9.57%	1.199%
12	14.530	1942	1947	1956	rBV4	9582	17923	1.41%	0.177%
13	14.642	1959	1966	1979	rVV	381622	632362	49.82%	6.245%
14	15.482	2103	2109	2114	rVB2	11270	15569	1.23%	0.154%
15	16.128	2211	2219	2233	rBV	357664	669457	52.74%	6.612%
16	16.346	2251	2256	2258	rBV4	13641	21727	1.71%	0.215%
17	17.133	2387	2390	2394	rBV3	15619	19580	1.54%	0.193%
18	17.192	2394	2400	2404	rVV4	9663	17526	1.38%	0.173%
19	17.386	2427	2433	2449	rBV	458942	755969	59.55%	7.466%
20	17.503	2449	2453	2458	rVB7	12338	20765	1.64%	0.205%
21	17.873	2510	2516	2520	rBV2	28036	39119	3.08%	0.386%
22	18.273	2580	2584	2589	rBV6	23257	38370	3.02%	0.379%
23	18.567	2628	2634	2638	rBV2	35737	50724	4.00%	0.501%
24	19.025	2708	2712	2716	rBV3	17005	24314	1.92%	0.240%
25	19.189	2737	2740	2744	rBV2	40979	50243	3.96%	0.496%
26	19.313	2759	2761	2765	rBV5	12887	12901	1.02%	0.127%
27	19.354	2765	2768	2769	rBV3	16580	16774	1.32%	0.166%
28	19.418	2775	2779	2780	rBV3	11554	14750	1.16%	0.146%
29	19.765	2836	2838	2842	rVB3	32374	33855	2.67%	0.334%
30	19.994	2872	2877	2886	rVB	943238	1269408	100.00%	12.537%
31	20.300	2926	2929	2933	rVB3	48858	58493	4.61%	0.578%
32	20.582	2975	2977	2978	rBV2	20939	14899	1.17%	0.147%
33	20.793	3010	3013	3016	rBV	45066	50453	3.97%	0.498%
34	21.293	3095	3098	3103	rBV	71217	89598	7.06%	0.885%

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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

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35	21.657	3154	3160	3169	rvB2	457467	855346	67.38%	8.447%
36	24.853	3696	3704	3720	rvB2	357951	1052671	82.93%	10.396%

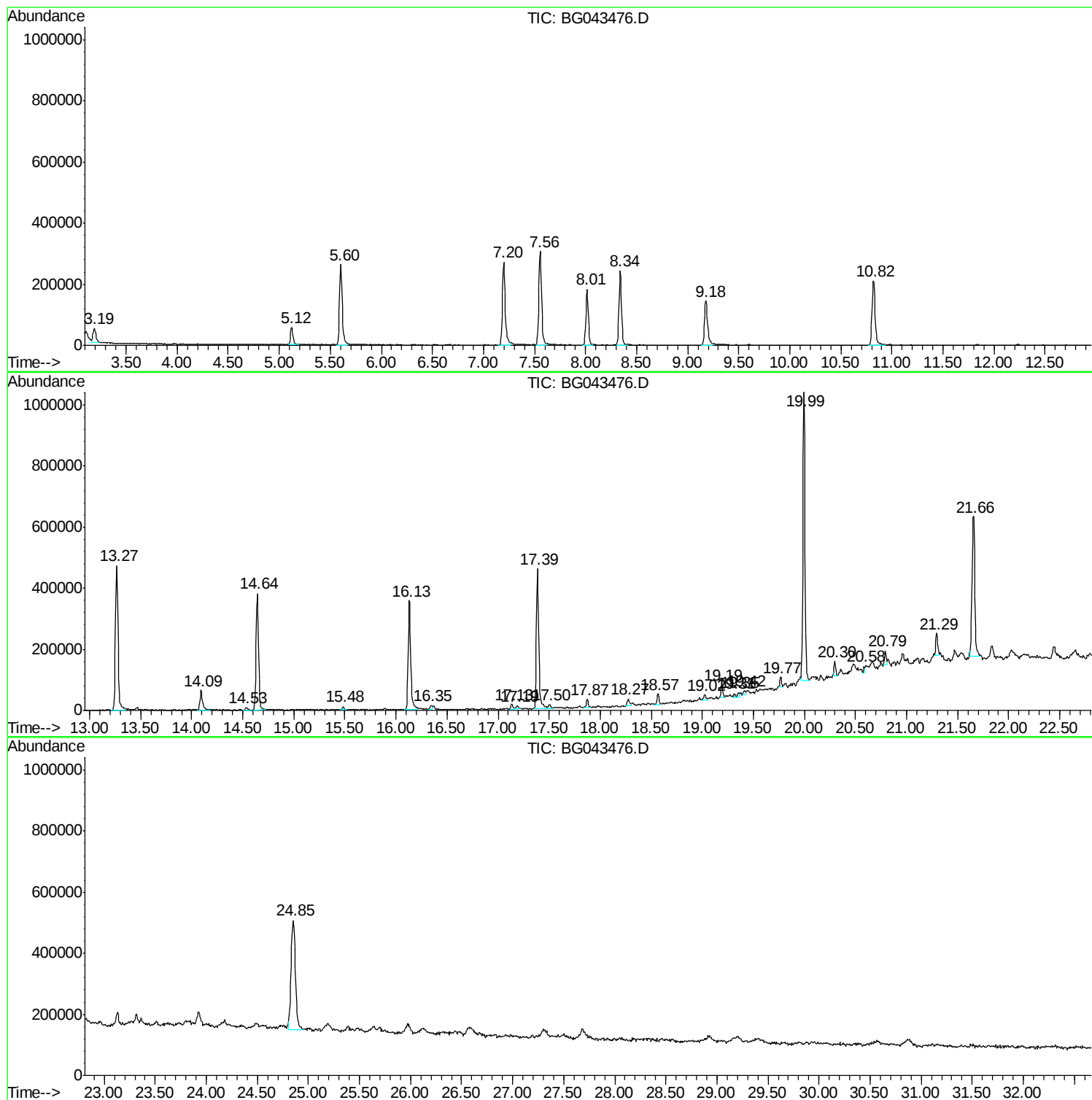
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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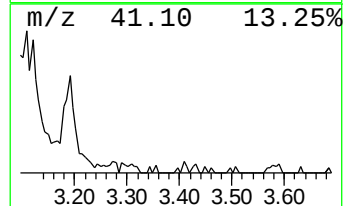
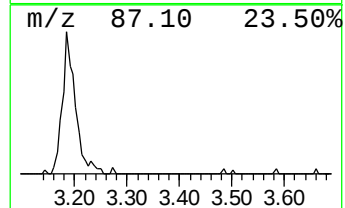
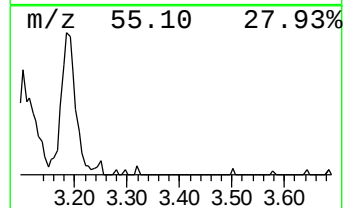
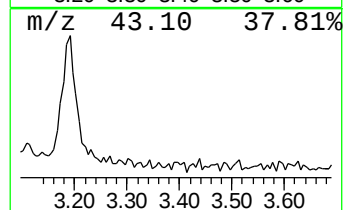
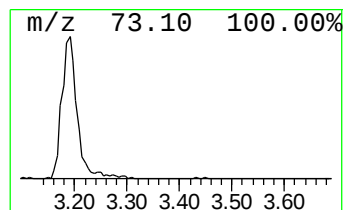
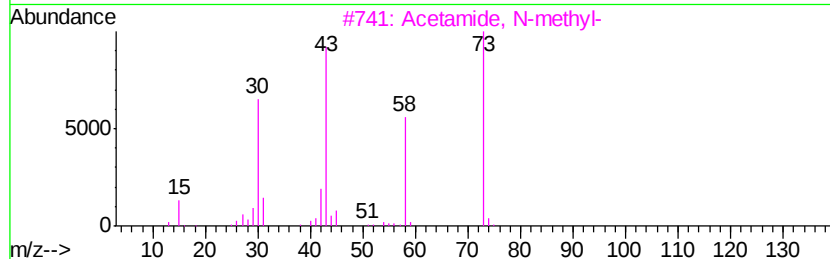
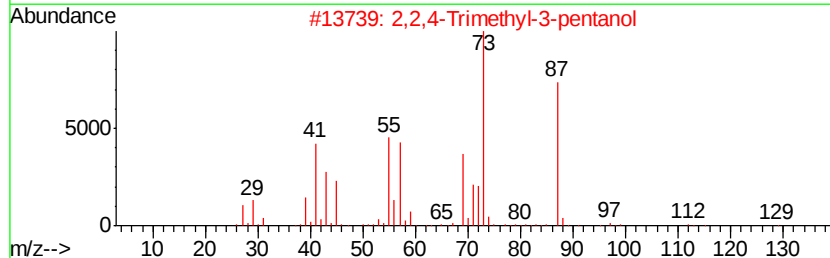
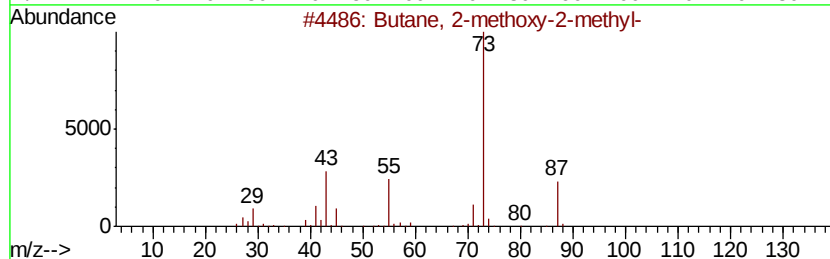
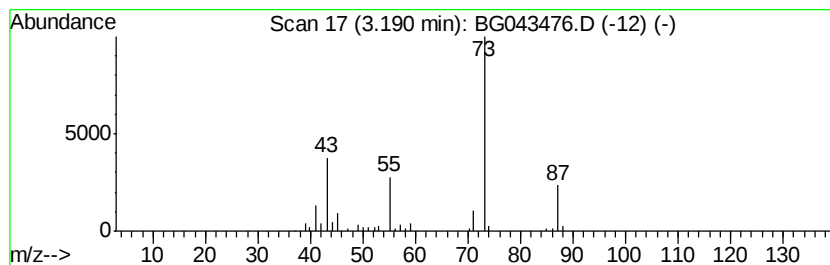
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	5.34 ng	86816	1,4-Dichlorobenzene-d4	8.01

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	40
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9



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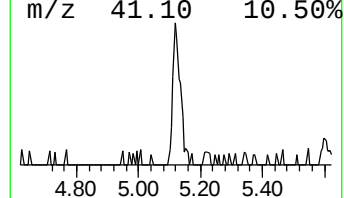
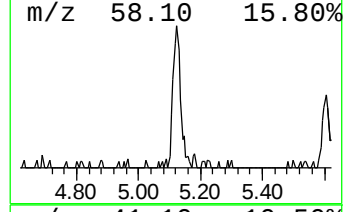
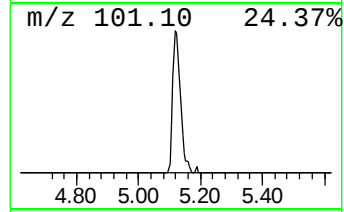
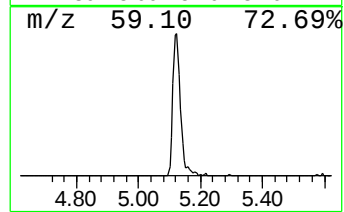
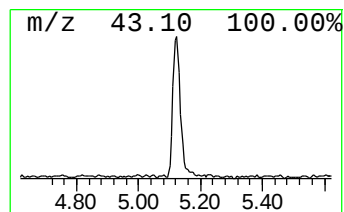
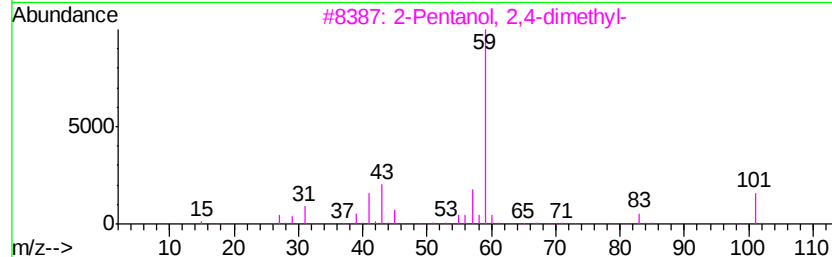
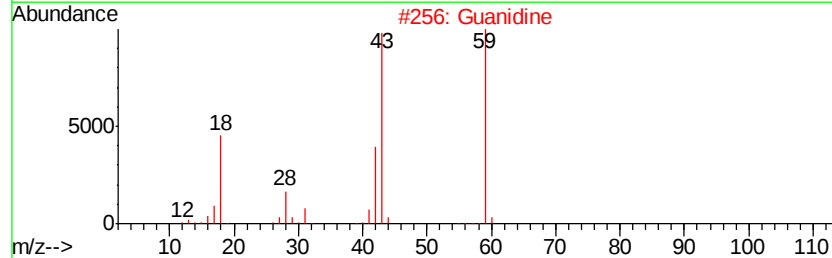
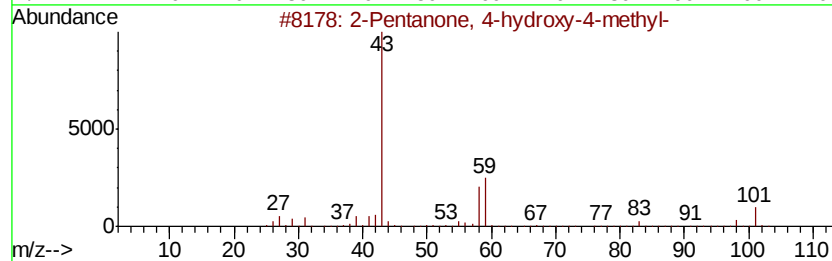
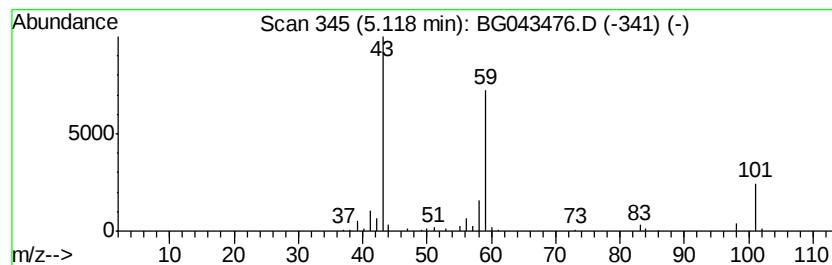
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	5.86 ng	95297	1,4-Dichlorobenzene-d4	8.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Guanidine	59	CH5N3	000113-00-8	43
3			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40
4			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17



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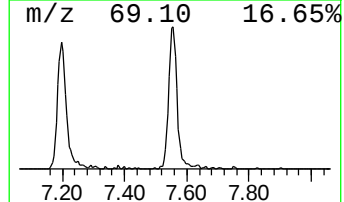
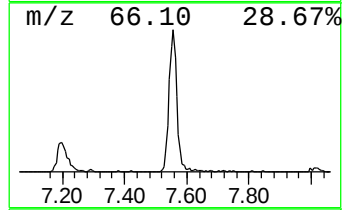
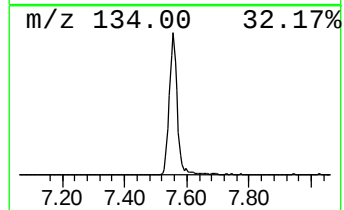
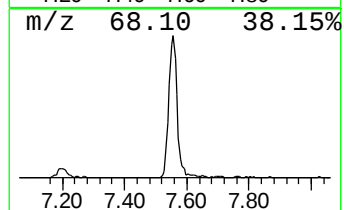
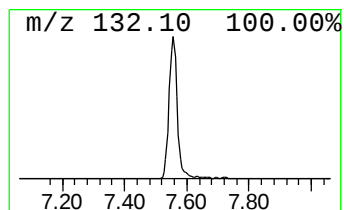
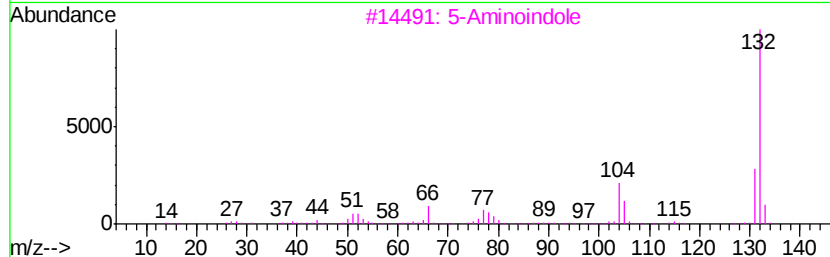
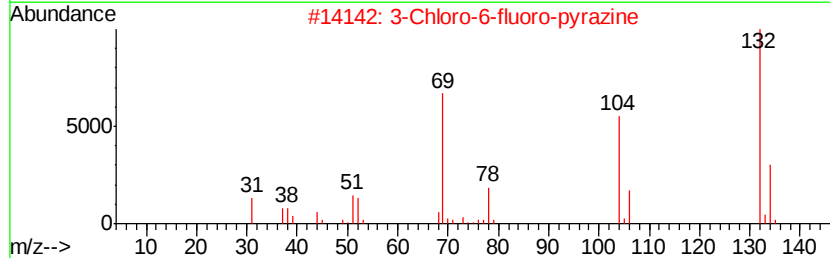
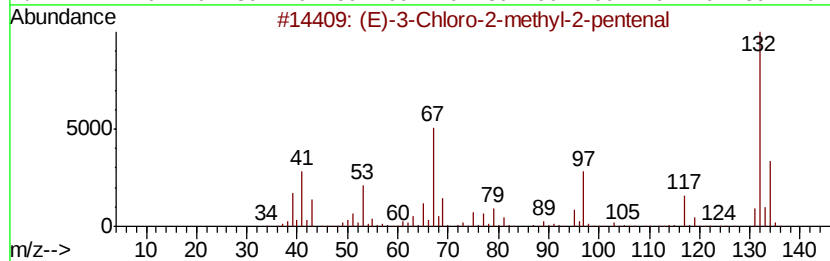
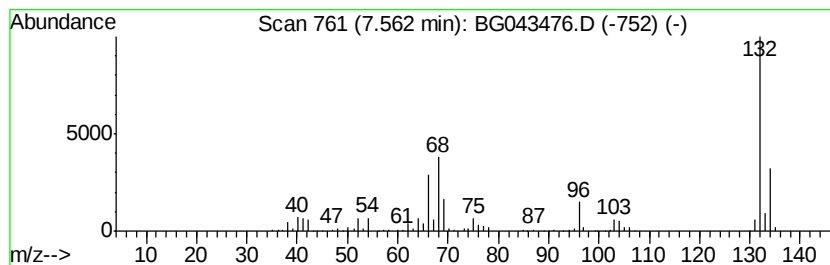
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Peak Number 3 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	34.63 ng	563203	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		N-(3,4-Methylenedioxyphenyl)isop...	267	C17H17NO2	1000378-96-6	10



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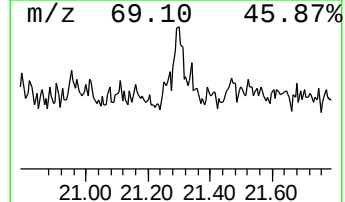
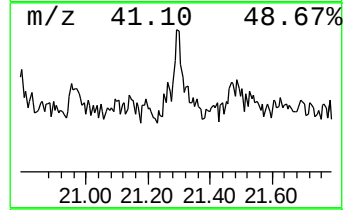
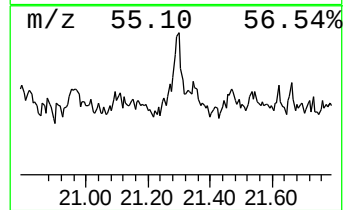
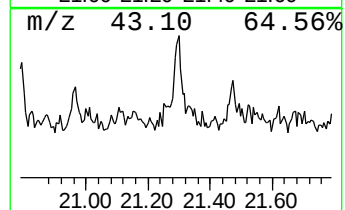
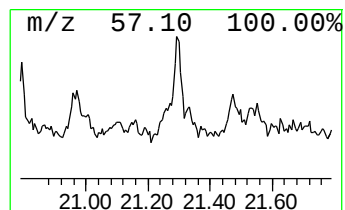
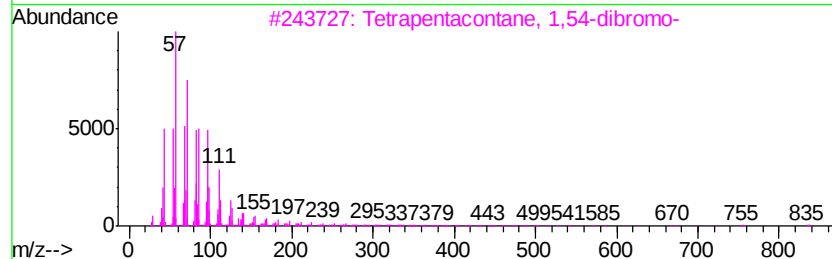
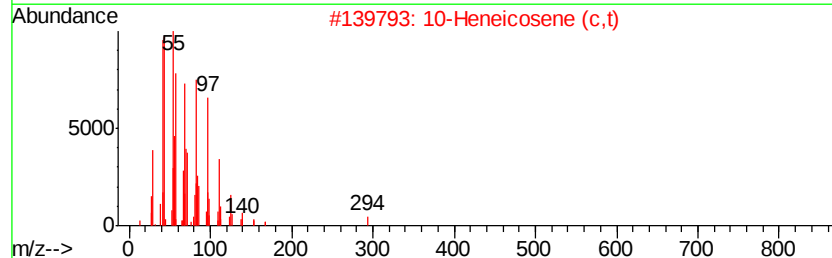
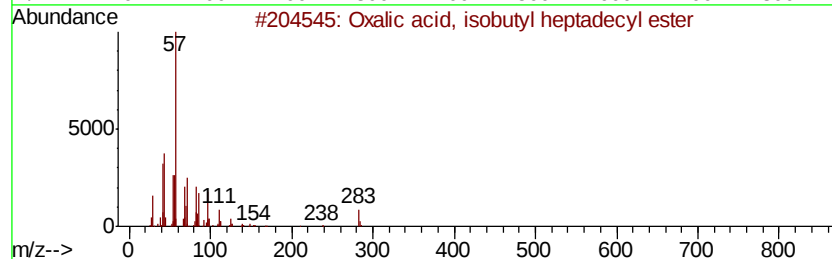
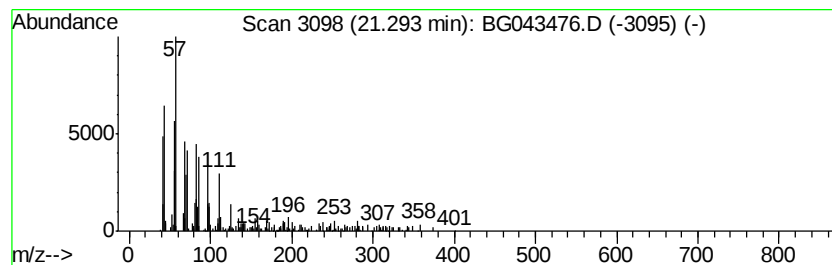
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Peak Number 5 Oxalic acid, isobutyl hepta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	2.10 ng	89598	Chrysene-d12	21.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	80
2		10-Heneicosene (c,t)	294	C21H42	095008-11-0	70
3		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	62
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	62
5		Cyclohexadecane	224	C16H32	000295-65-8	60



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.19	5.3	ng	86816	1	8.01	325310	20.0
2-Pentanone, 4-hy...	5.12	5.9	ng	95297	1	8.01	325310	20.0
unknown7.56	7.56	34.6	ng	563203	1	8.01	325310	20.0
Oxalic acid, isob...	21.29	2.1	ng	89598	5	21.65	855346	20.0