

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP010820\
 Data File : BP001572.D
 Acq On : 09 Jan 2020 02:28
 Operator : JU
 Sample : L1051-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-3G-(11-13)

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:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.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	2.899	14	19	28	rBV	35024	67817	2.29%	0.433%
2	2.975	28	32	46	rVB	140410	214206	7.22%	1.368%
3	4.828	342	347	356	rBV	167641	243267	8.20%	1.553%
4	5.287	419	425	435	rVB	674693	994095	33.50%	6.347%
5	6.857	684	692	701	rBV	831915	1323352	44.59%	8.450%
6	7.204	743	751	758	rBV	768262	1202717	40.53%	7.679%
7	7.657	821	828	837	rVB	146895	226334	7.63%	1.445%
8	7.975	874	882	890	rBV	584307	909026	30.63%	5.804%
9	8.804	1014	1023	1034	rBV	529280	844927	28.47%	5.395%
10	10.434	1292	1300	1310	rVB	193543	313096	10.55%	1.999%
11	12.922	1716	1723	1733	rVB	1250881	1795619	60.51%	11.465%
12	13.769	1861	1867	1875	rBV	43888	62827	2.12%	0.401%
13	14.298	1951	1957	1966	rBV	303700	454720	15.32%	2.903%
14	15.804	2206	2213	2227	rBV	1111498	1624473	54.74%	10.372%
15	17.063	2420	2427	2438	rVB	444628	616108	20.76%	3.934%
16	17.992	2581	2585	2593	rBV	43119	62558	2.11%	0.399%
17	19.092	2767	2772	2774	rBV4	22558	35972	1.21%	0.230%
18	19.121	2774	2777	2788	rVB2	66457	106617	3.59%	0.681%
19	19.239	2793	2797	2808	rVB2	29488	48954	1.65%	0.313%
20	19.651	2861	2867	2872	rBV	2435511	2967652	100.00%	18.949%
21	20.915	3078	3082	3087	rBV3	50096	65216	2.20%	0.416%
22	21.162	3119	3124	3133	rBV2	562681	706214	23.80%	4.509%
23	21.351	3153	3156	3159	rVB	35795	34943	1.18%	0.223%
24	21.792	3228	3231	3235	rVB2	38466	47803	1.61%	0.305%
25	22.786	3397	3400	3407	rVB3	42261	59656	2.01%	0.381%
26	23.409	3500	3506	3514	rVB	310787	633369	21.34%	4.044%

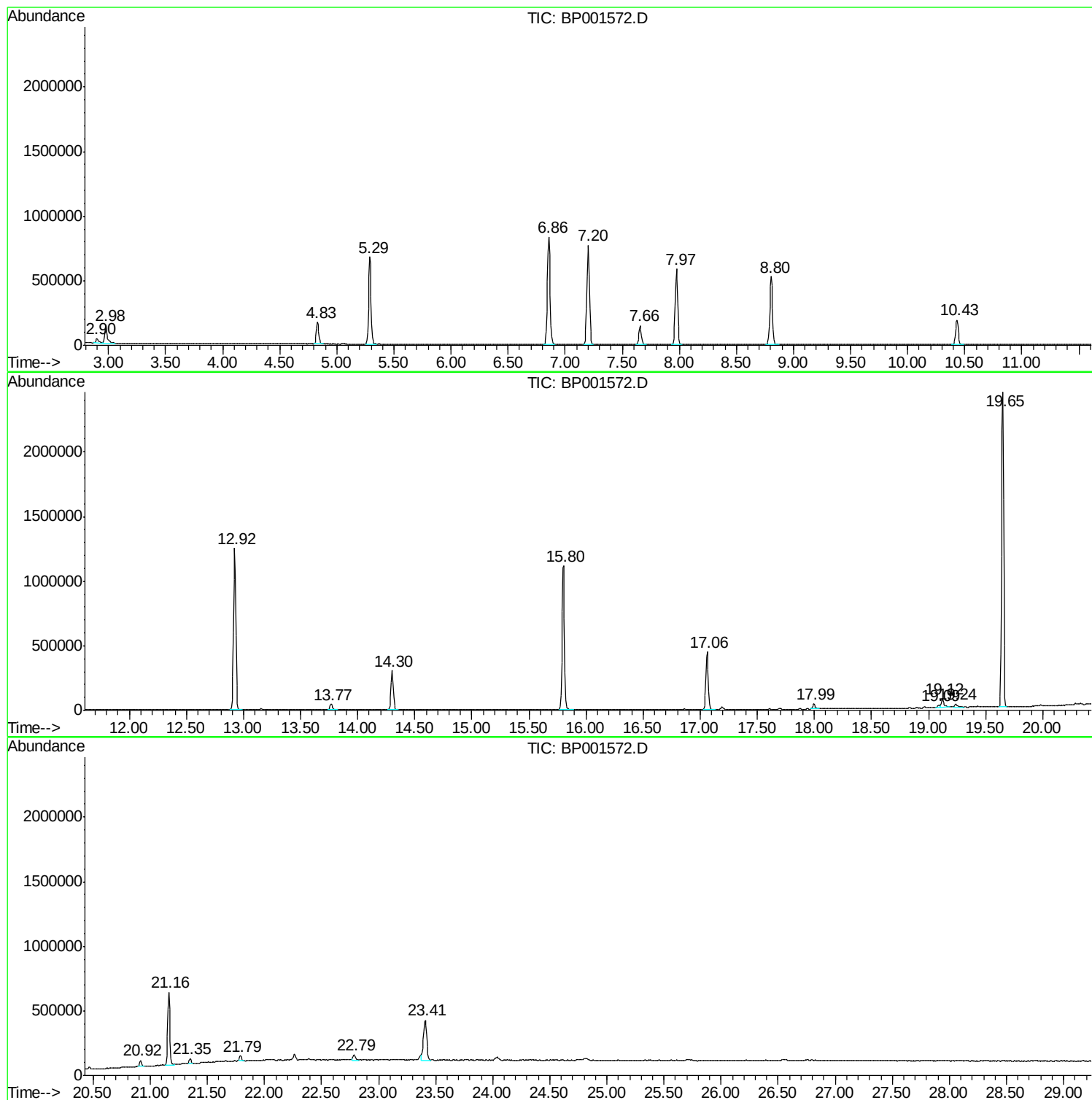
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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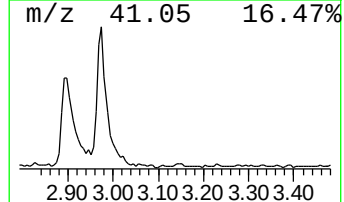
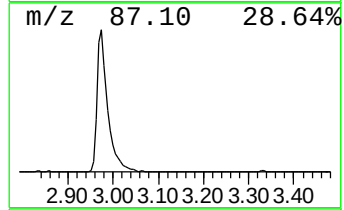
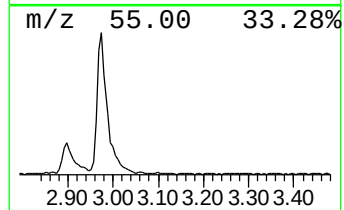
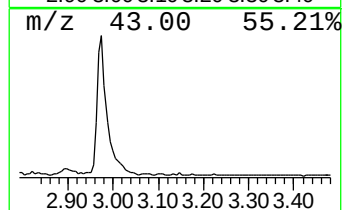
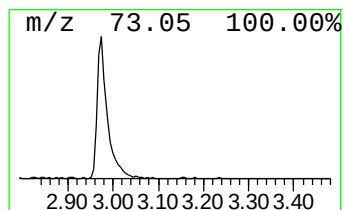
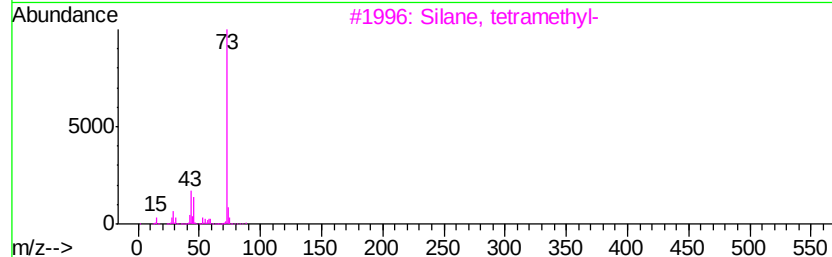
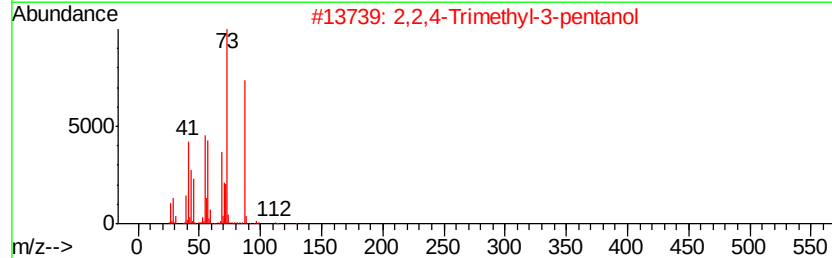
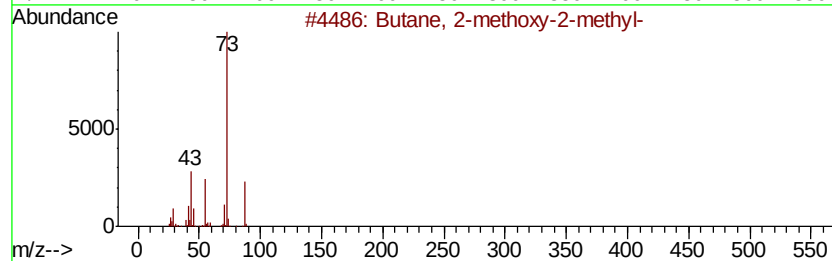
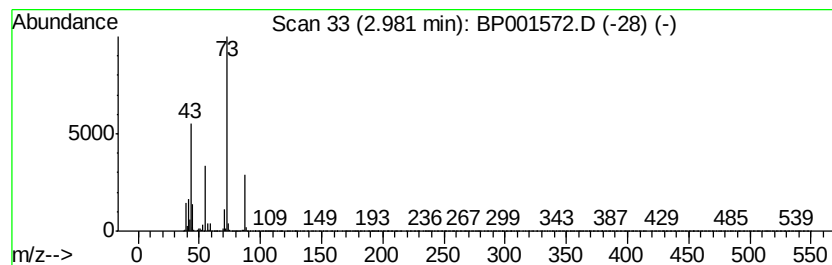
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	18.93 ng	214206	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4		Pentanoic acid, 2-hydroxy-4-meth...	146	C7H14O3	040348-72-9	25
5		Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	23



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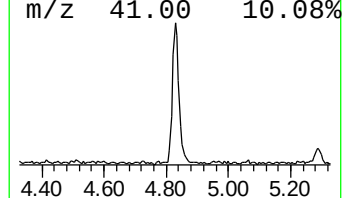
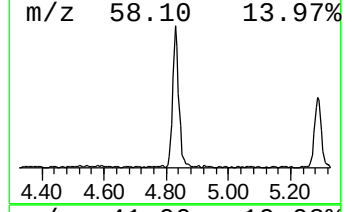
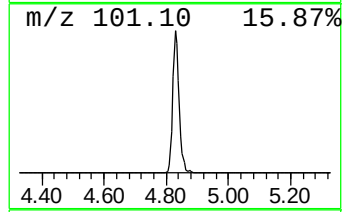
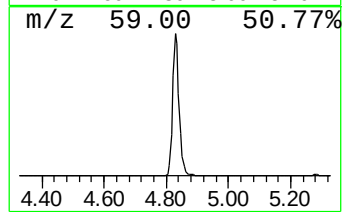
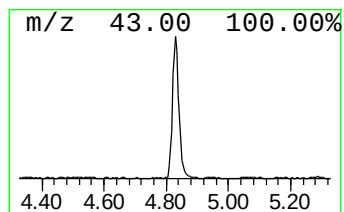
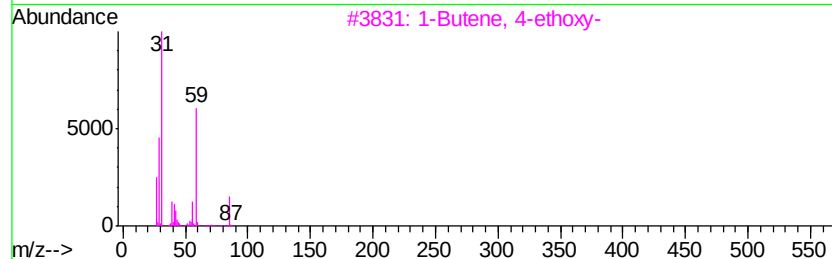
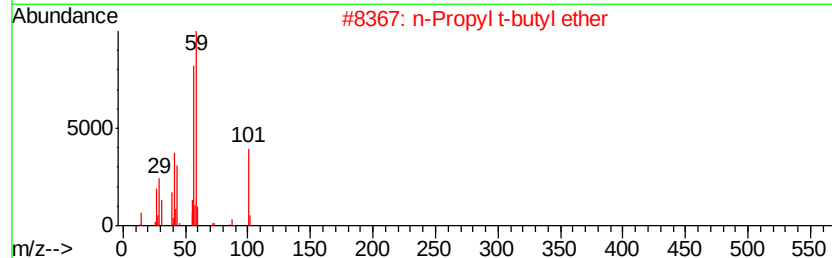
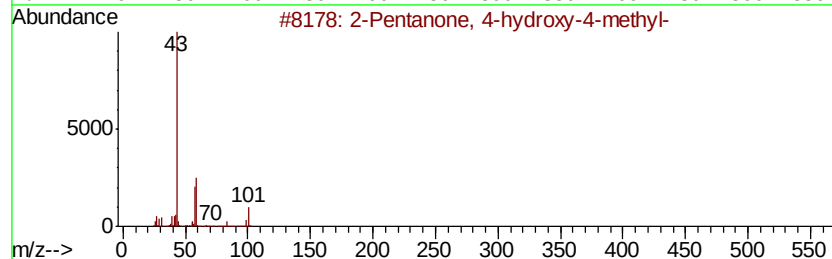
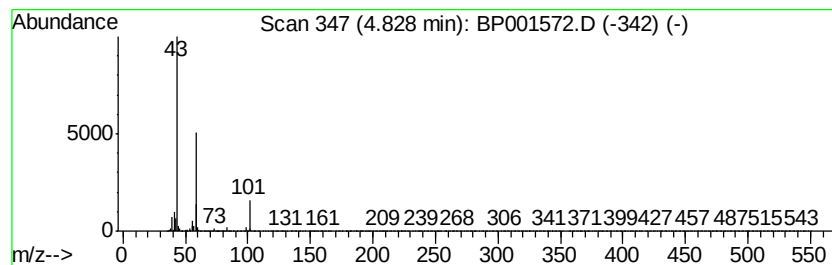
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	21.50 ng	243267	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3		1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23
4		Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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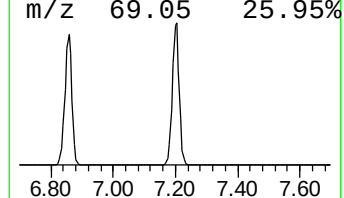
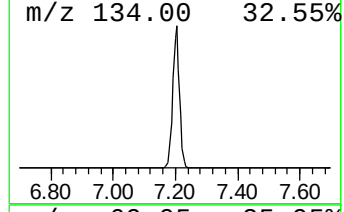
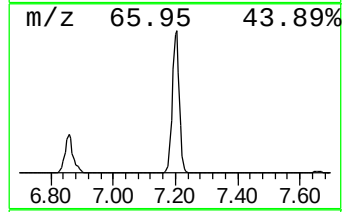
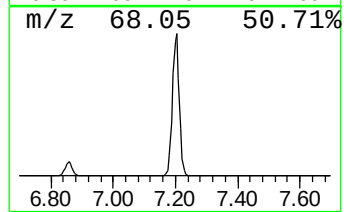
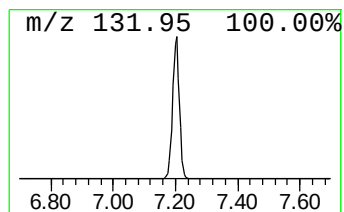
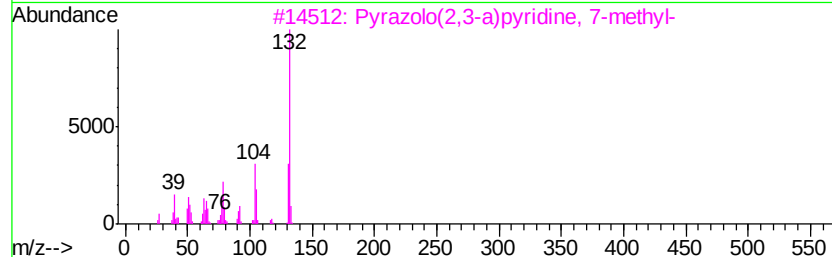
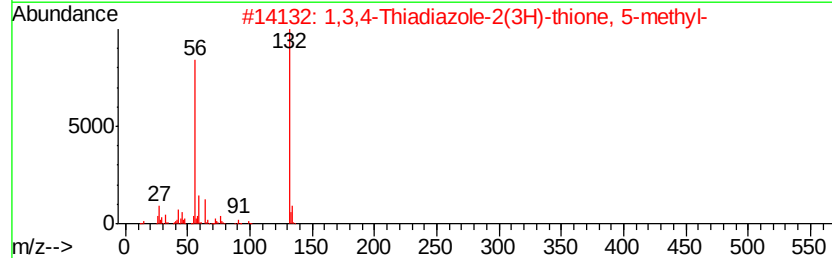
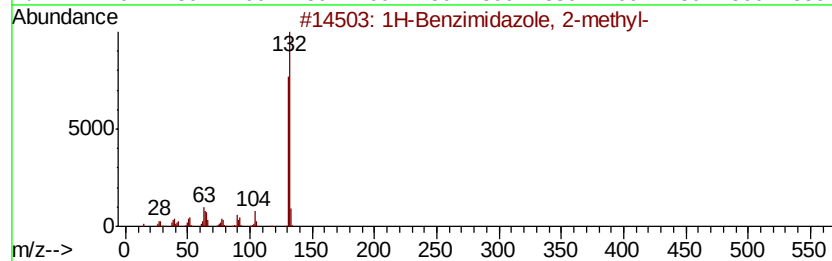
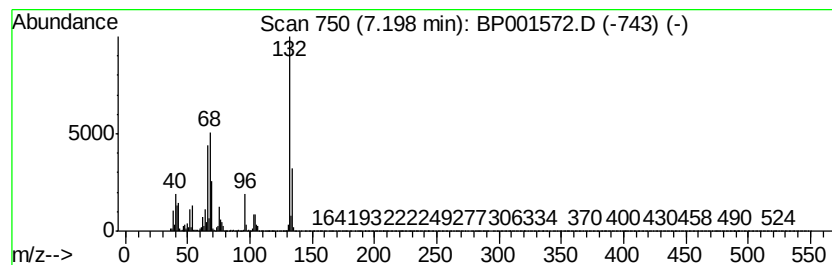
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Peak Number 4 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	106.28 ng	1202720	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		Pvrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	14
4		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14



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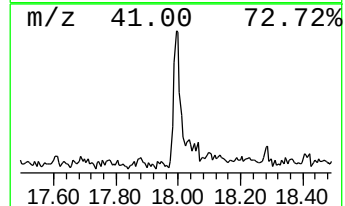
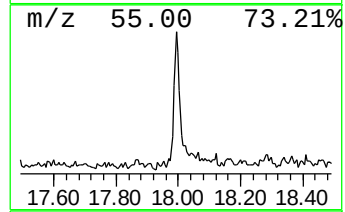
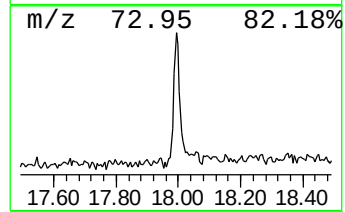
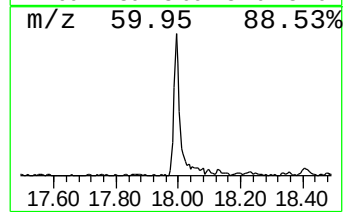
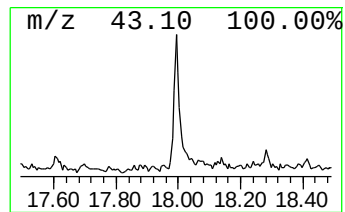
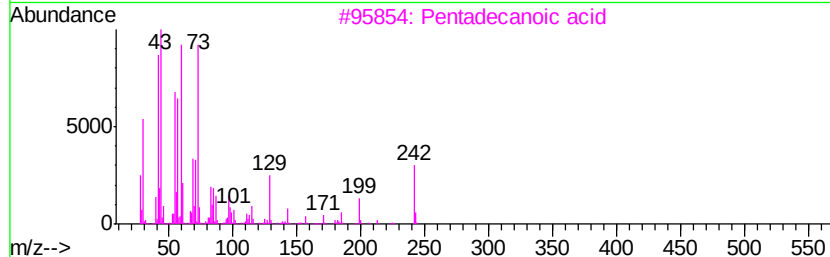
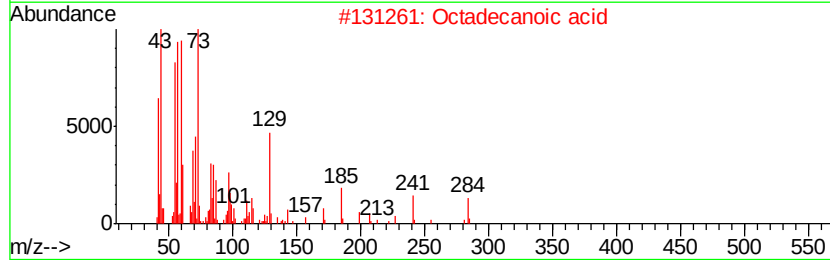
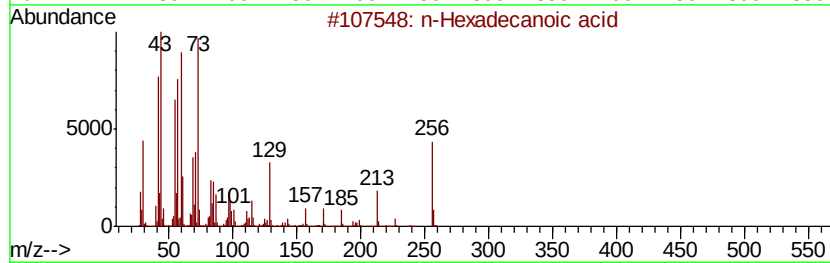
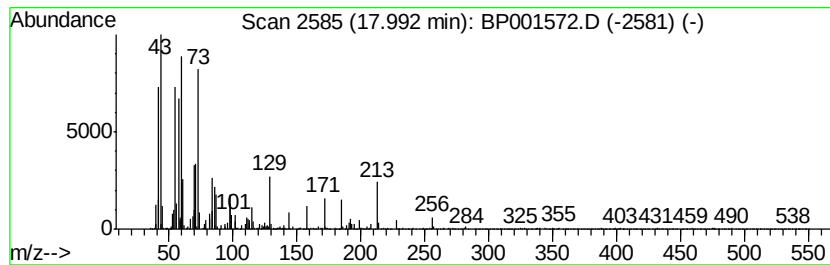
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.99	2.03 ng	62558	Phenanthrene-d10	17.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	Octadecanoic acid	284	C18H36O2	000057-11-4	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	59



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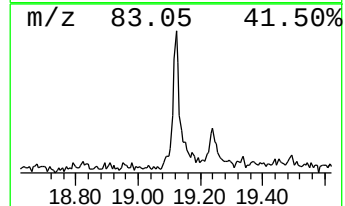
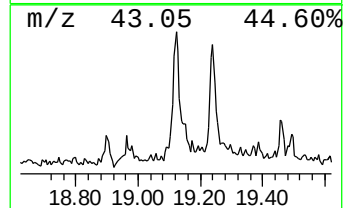
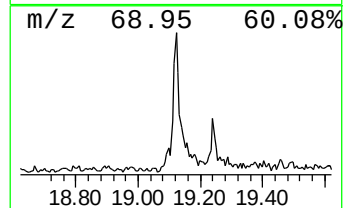
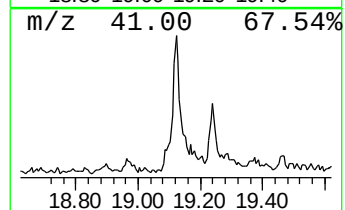
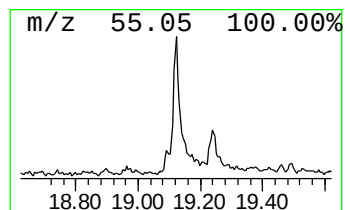
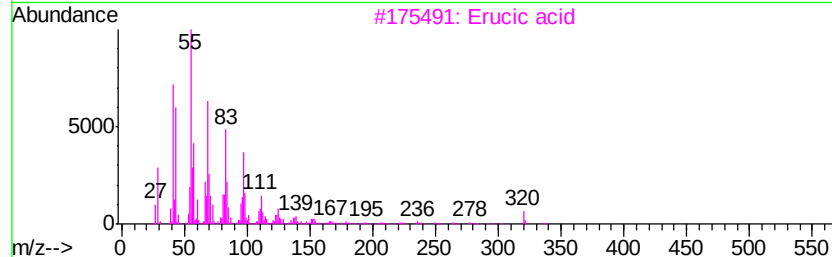
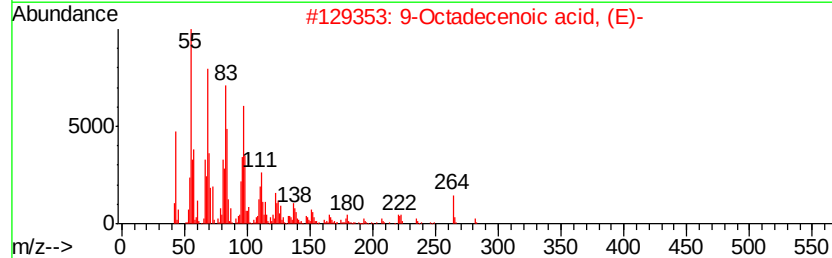
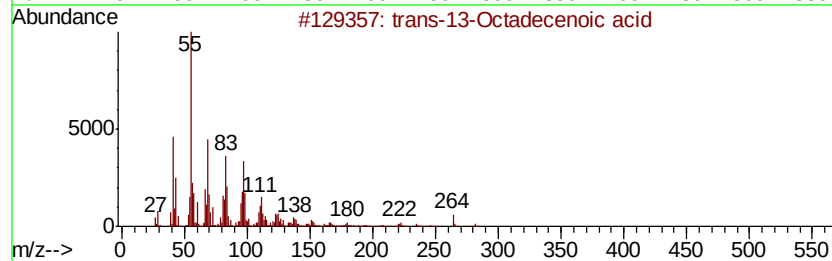
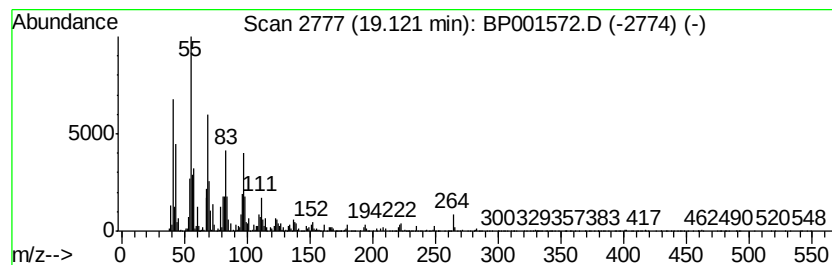
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 trans-13-Octadecenoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	3.02 ng	106617	Chrysene-d12	21.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	95
2		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	95
3		Erucic acid	338	C22H42O2	000112-86-7	81
4		9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	68
5		14-Pentadecenoic acid	240	C15H28O2	017351-34-7	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.98	18.9	ng	214206	1	7.66	226334	20.0
2-Pentanone, 4-hy...	4.83	21.5	ng	243267	1	7.66	226334	20.0
unknown7.20	7.20	106.3	ng	1202720	1	7.66	226334	20.0
n-Hexadecanoic acid	17.99	2.0	ng	62558	4	17.06	616108	20.0
trans-13-Octadece...	19.12	3.0	ng	106617	5	21.16	706214	20.0