

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP010920\
 Data File : BP001577.D
 Acq On : 09 Jan 2020 13:45
 Operator : JU
 Sample : PB125970BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PB125970BL

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_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	2.975	28	32	44	rVB	83647	109652	3.50%	0.715%
2	4.828	342	347	359	rVB	148203	216589	6.91%	1.413%
3	5.293	419	426	436	rVB	662272	993837	31.69%	6.482%
4	6.858	684	692	707	rBV	771312	1208524	38.53%	7.883%
5	7.205	743	751	764	rBV	732379	1119698	35.70%	7.303%
6	7.657	822	828	836	rBV	155779	246351	7.85%	1.607%
7	7.981	875	883	891	rVB	549161	862536	27.50%	5.626%
8	8.810	1013	1024	1034	rBV	472937	782924	24.96%	5.107%
9	10.434	1292	1300	1308	rBV	204641	336434	10.73%	2.194%
10	12.928	1717	1724	1737	rVB	1194835	1739283	55.45%	11.345%
11	13.769	1863	1867	1875	rBV	21331	33078	1.05%	0.216%
12	14.304	1951	1958	1968	rBV	348561	499727	15.93%	3.259%
13	15.804	2206	2213	2226	rBV	1192472	1631356	52.01%	10.641%
14	17.063	2420	2427	2439	rVB	471406	672645	21.45%	4.387%
15	17.998	2580	2586	2593	rBV3	47333	71164	2.27%	0.464%
16	18.833	2724	2728	2734	rBV3	24278	36018	1.15%	0.235%
17	19.657	2861	2868	2874	rBV	2350381	3136430	100.00%	20.458%
18	20.916	3078	3082	3095	rBV	137062	197224	6.29%	1.286%
19	21.169	3120	3125	3130	rBV	615185	744522	23.74%	4.856%
20	22.392	3330	3333	3340	rVB	38580	53899	1.72%	0.352%
21	23.410	3500	3506	3514	rVB2	330973	639527	20.39%	4.171%

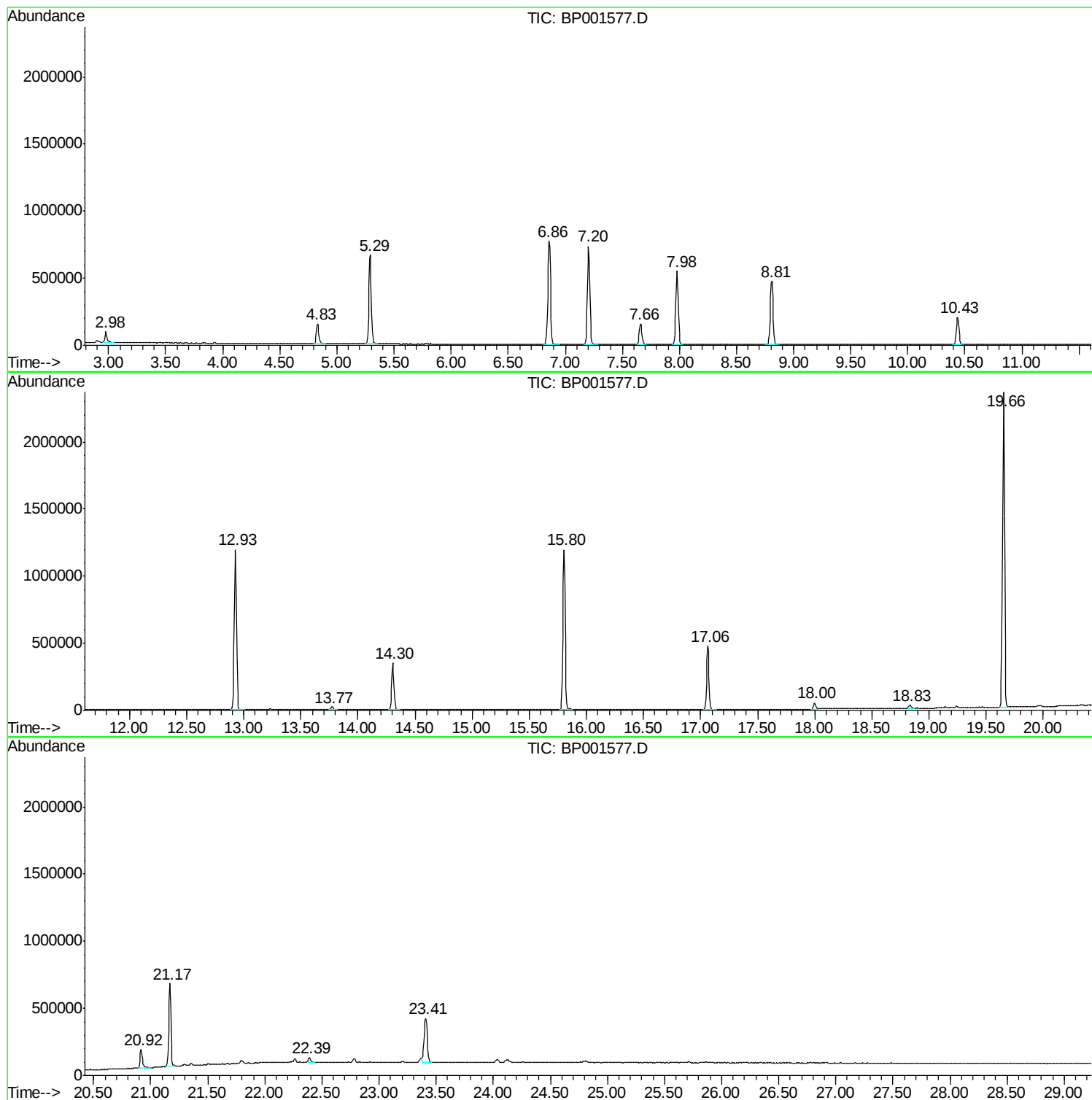
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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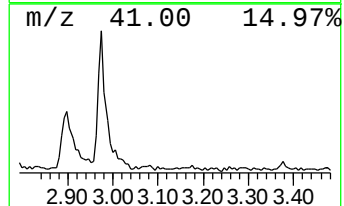
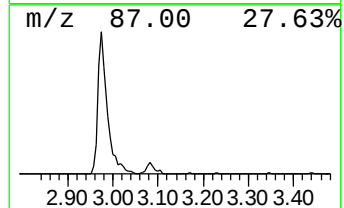
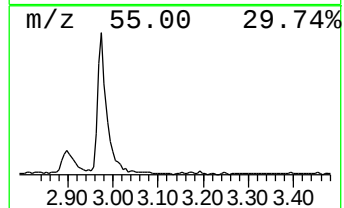
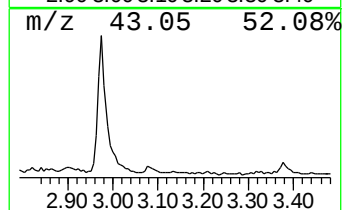
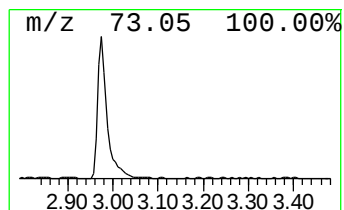
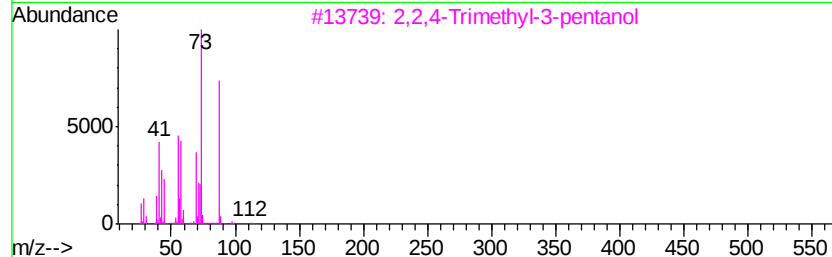
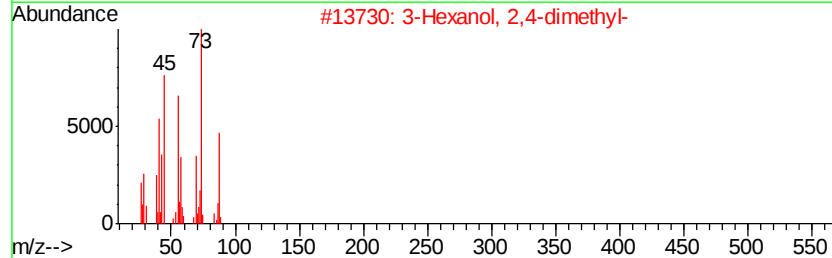
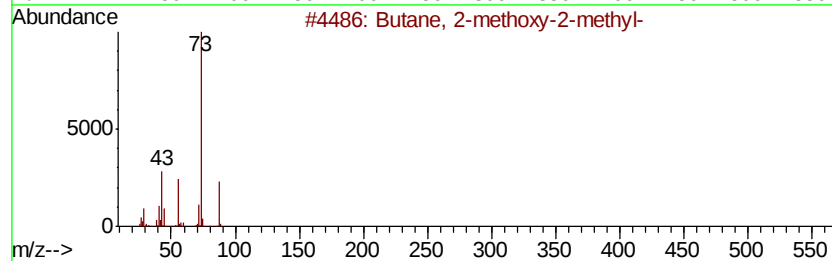
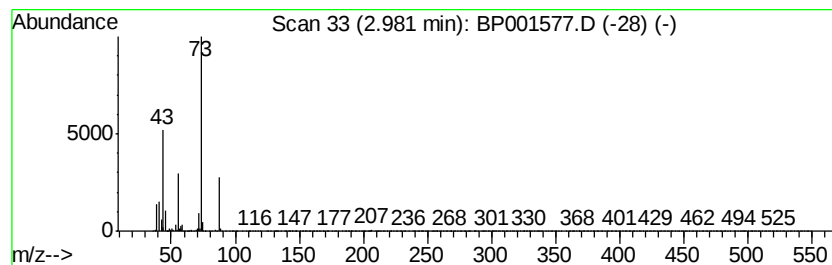
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	8.90 ng	109652	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	90
2		3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	45
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	35
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	23



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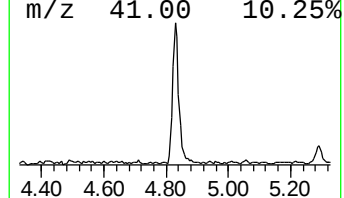
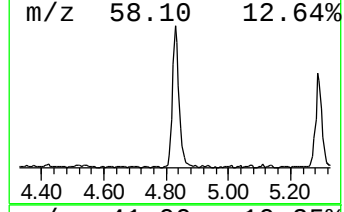
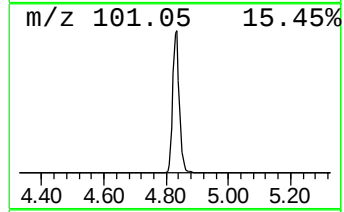
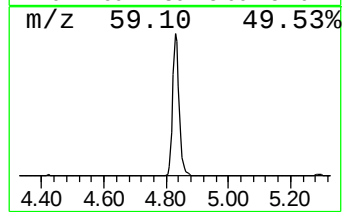
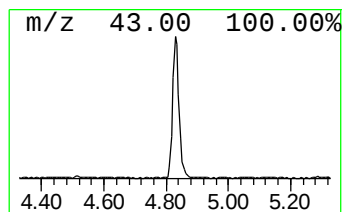
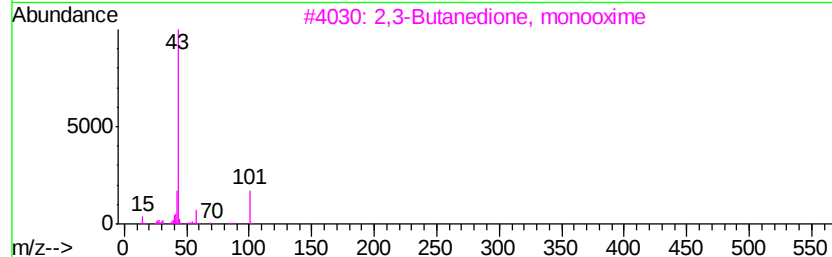
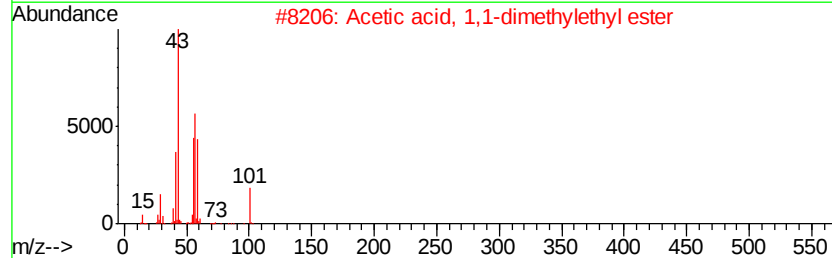
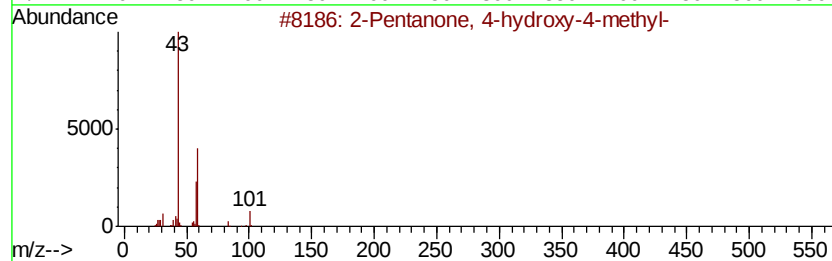
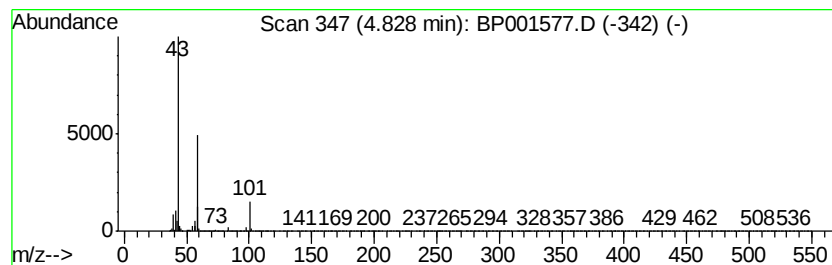
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	17.58 ng	216589	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	38
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9



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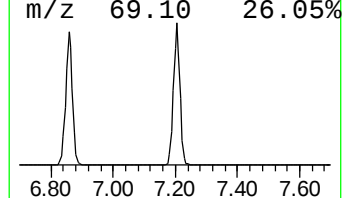
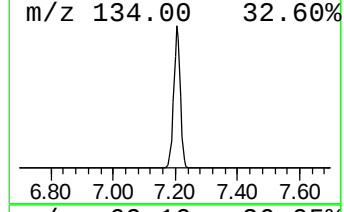
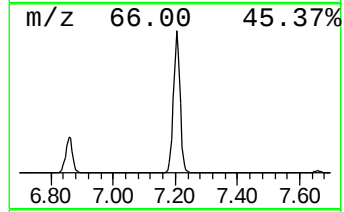
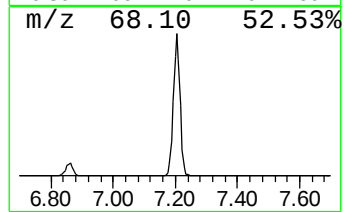
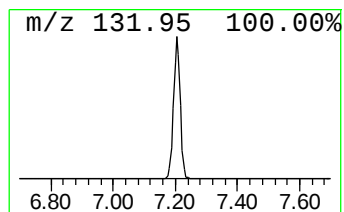
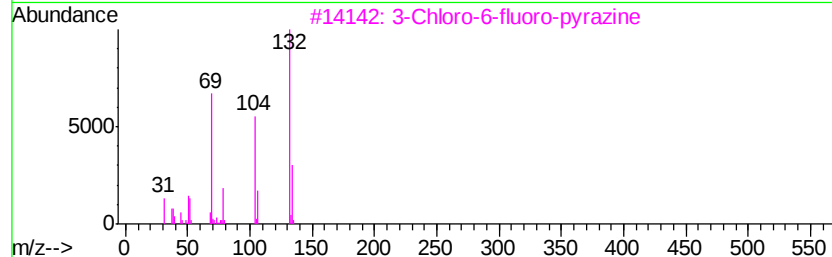
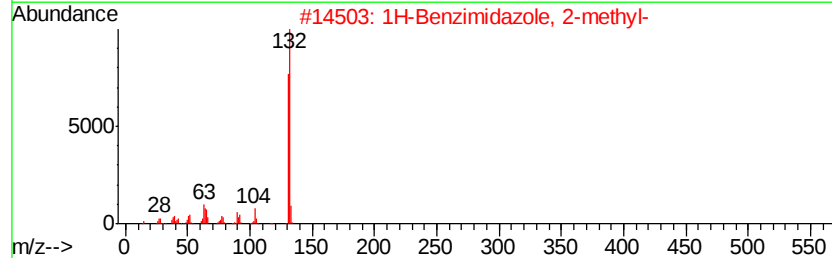
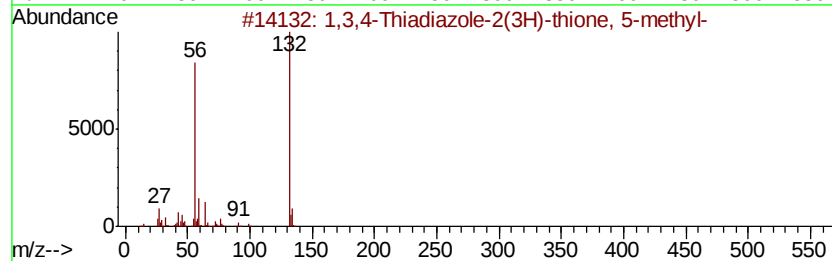
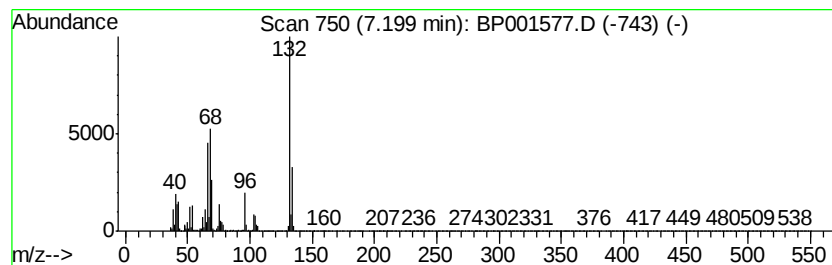
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Peak Number 3 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	90.90 ng	1119700	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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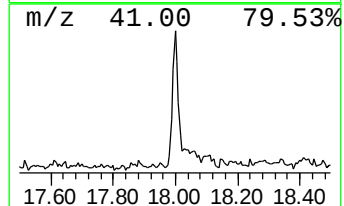
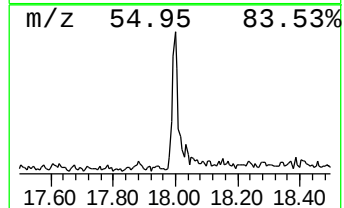
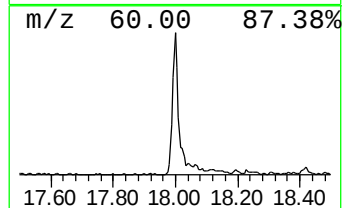
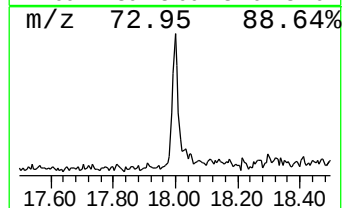
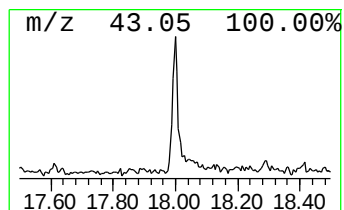
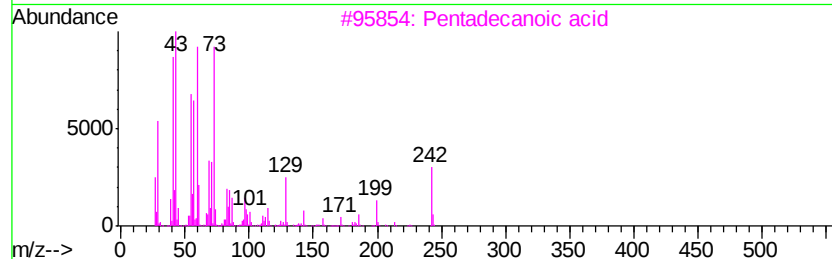
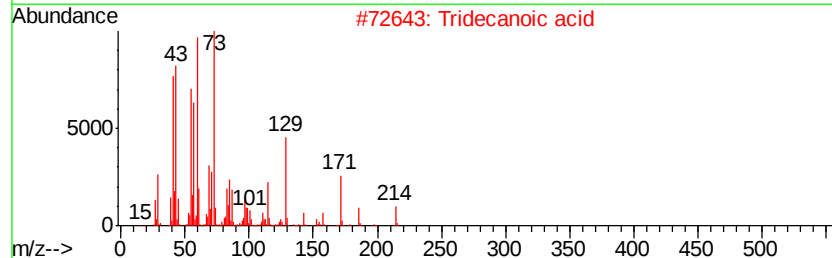
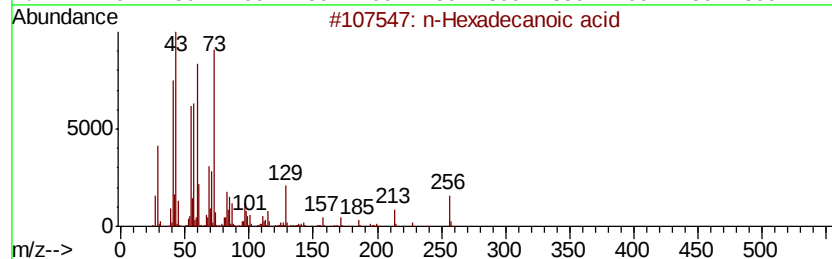
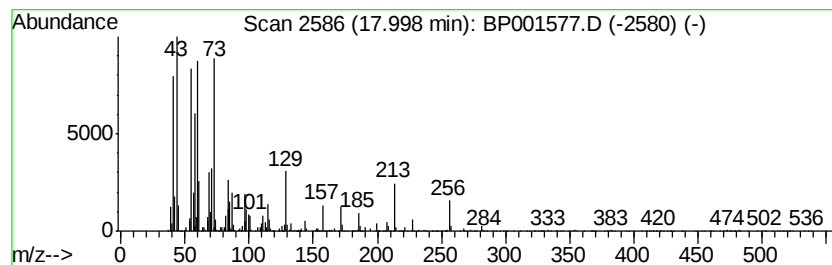
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.00	2.12 ng	71164	Phenanthrene-d10	17.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	92
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	62
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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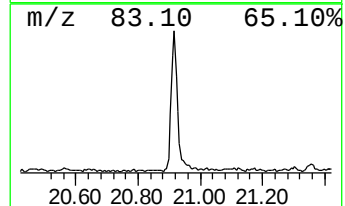
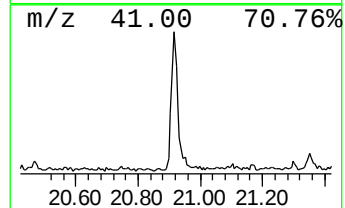
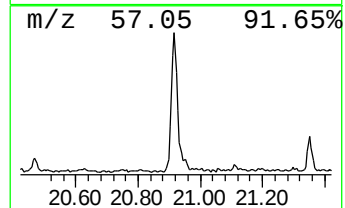
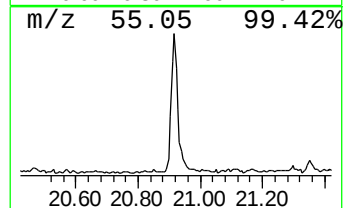
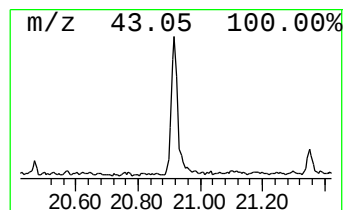
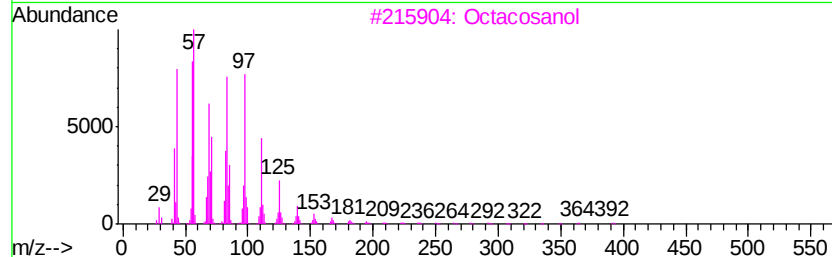
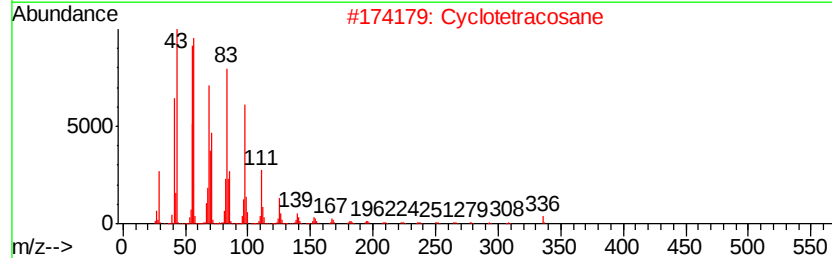
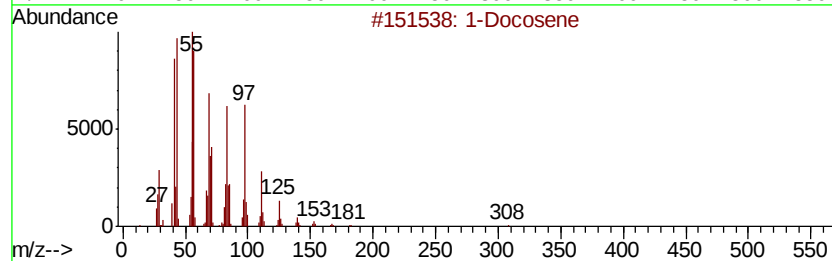
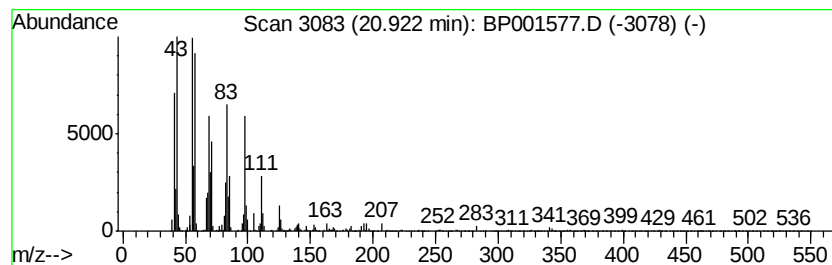
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.92	5.30 ng	197224	Chrysene-d12	21.17

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	98
2	Cyclotetracosane		336	C24H48	000297-03-0	94
3	Octacosanol		410	C28H58O	000557-61-9	94
4	Fumaric acid, 2-chloropropyl dod...		360	C19H33ClO4	1000348-57-0	93
5	2-Chloropropionic acid, octadec...		360	C21H41ClO2	088104-31-8	93



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.98	8.9	ng	109652	1	7.66	246351	20.0
2-Pentanone, 4-hy...	4.83	17.6	ng	216589	1	7.66	246351	20.0
unknown7.20	7.20	90.9	ng	1119700	1	7.66	246351	20.0
n-Hexadecanoic acid	18.00	2.1	ng	71164	4	17.06	672645	20.0
1-Docosene	20.92	5.3	ng	197224	5	21.17	744522	20.0