

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
 Data File : BF134138.D
 Acq On : 07 Jul 2023 15:15
 Operator : CG\JU
 Sample : 03392-05
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SRY-3

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_F\Methods\8270-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134138.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	18	rVB	1166935	1526183	64.93%	7.539%
2	2.240	23	26	31	rVB	30370	35511	1.51%	0.175%
3	5.087	506	510	523	rBV	69651	101601	4.32%	0.502%
4	5.481	572	577	580	rBV	2214897	2090782	88.94%	10.328%
5	6.481	743	747	750	rBV	2153911	2047542	87.10%	10.115%
6	6.845	805	809	818	rBV	748872	637238	27.11%	3.148%
7	7.404	900	904	908	rBV	1403350	1354625	57.63%	6.692%
8	8.122	1023	1026	1034	rBV	978578	774506	32.95%	3.826%
9	9.198	1205	1209	1213	rBV	2683819	2350661	100.00%	11.612%
10	9.739	1298	1301	1305	rVB	45620	41823	1.78%	0.207%
11	9.880	1321	1325	1329	rBV	953774	752188	32.00%	3.716%
12	10.086	1355	1360	1364	rBV	27534	34019	1.45%	0.168%
13	10.598	1443	1447	1455	rVB	197562	169259	7.20%	0.836%
14	10.675	1456	1460	1468	rBV	1378468	1222539	52.01%	6.039%
15	10.798	1477	1481	1487	rVB3	42845	57716	2.46%	0.285%
16	10.986	1509	1513	1516	rBV5	24645	39419	1.68%	0.195%
17	11.269	1559	1561	1566	rVB4	35428	39579	1.68%	0.196%
18	11.374	1575	1579	1581	rBV	757779	631441	26.86%	3.119%
19	11.398	1581	1583	1586	rVV	257569	196148	8.34%	0.969%
20	11.451	1589	1592	1594	rVV	59867	49305	2.10%	0.244%
21	11.880	1662	1665	1666	rBV	32117	31779	1.35%	0.157%
22	11.904	1666	1669	1673	rVV	394071	384945	16.38%	1.902%
23	11.939	1673	1675	1681	rVB	77130	73946	3.15%	0.365%
24	11.992	1681	1684	1686	rBV2	56126	56271	2.39%	0.278%
25	12.204	1718	1720	1722	rVB2	43411	33909	1.44%	0.168%
26	12.598	1783	1787	1790	rBV	631061	572475	24.35%	2.828%
27	12.698	1801	1804	1808	rBV2	192646	186297	7.93%	0.920%
28	12.827	1820	1826	1829	rBV	599481	609005	25.91%	3.008%
29	12.974	1847	1851	1856	rVB	2102954	1934703	82.30%	9.557%
30	14.039	2027	2032	2034	rBV2	637860	868631	36.95%	4.291%
31	14.063	2034	2036	2041	rVB	297482	245186	10.43%	1.211%
32	15.098	2209	2212	2216	rBV	241298	369979	15.74%	1.828%
33	15.480	2274	2277	2284	rVB	256225	364631	15.51%	1.801%
34	15.545	2285	2288	2292	rVV	309768	359114	15.28%	1.774%

Sum of corrected areas: 20242956

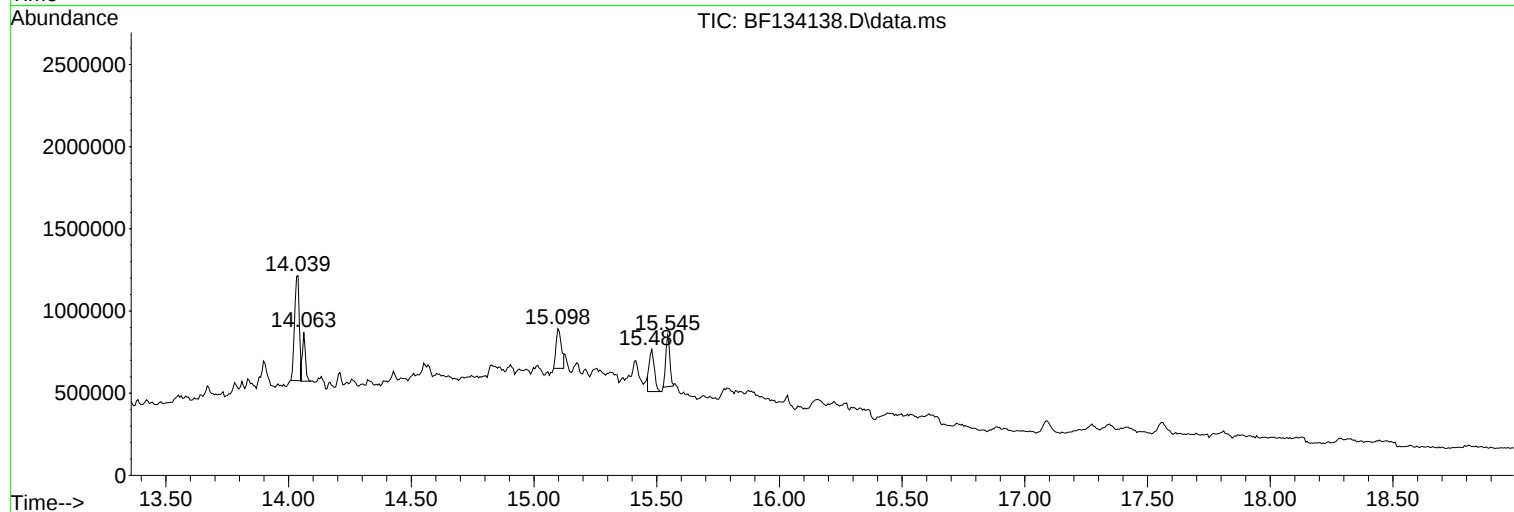
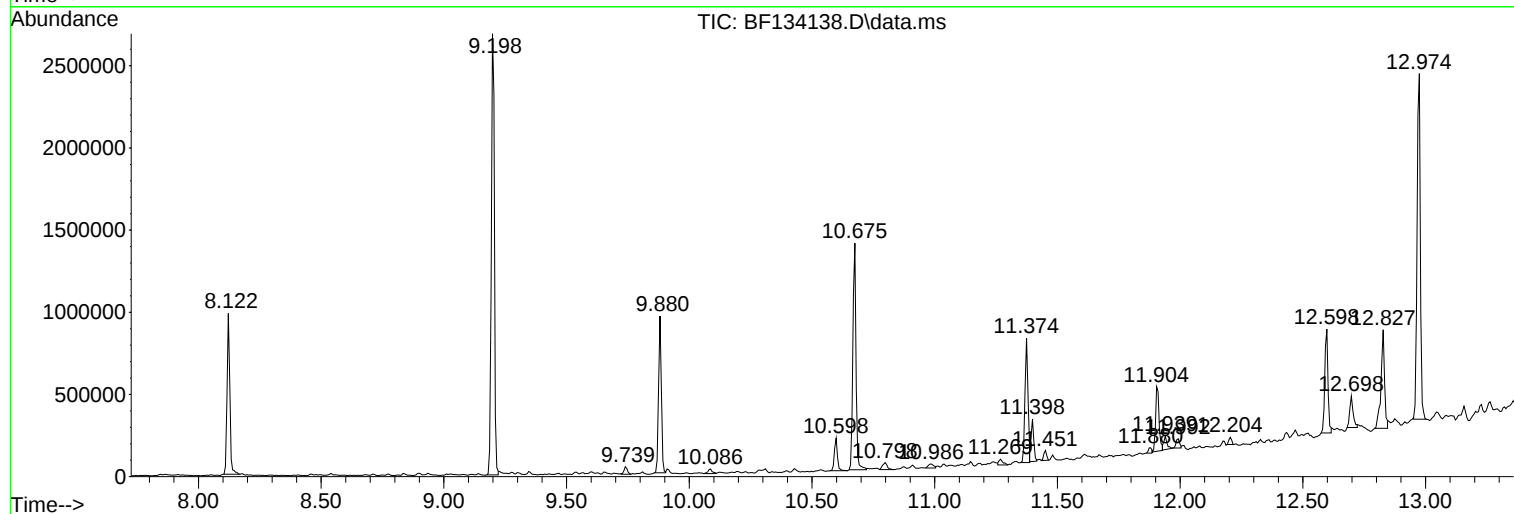
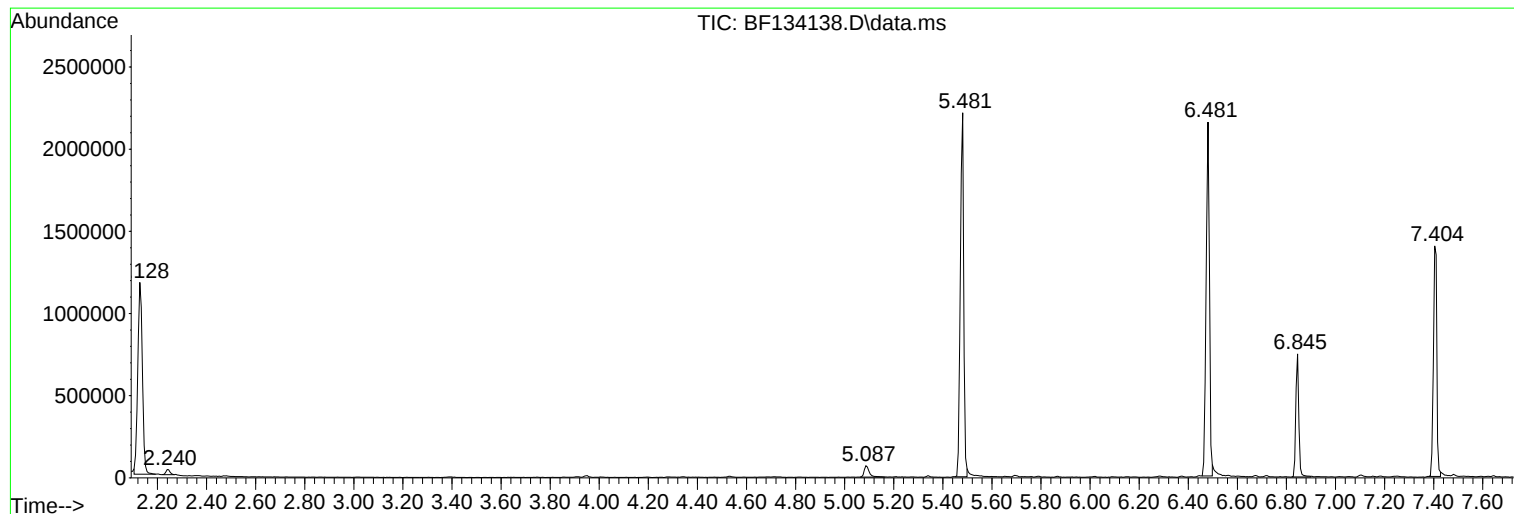
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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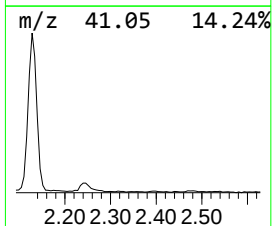
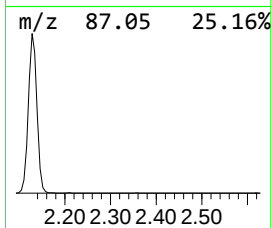
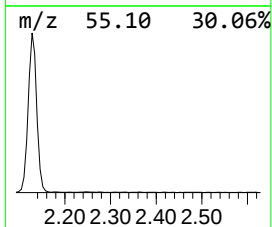
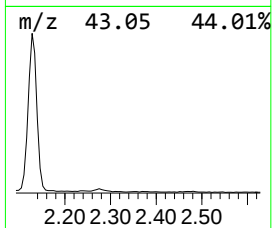
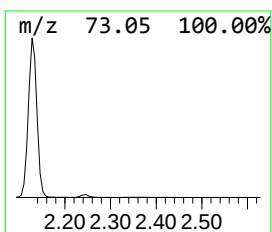
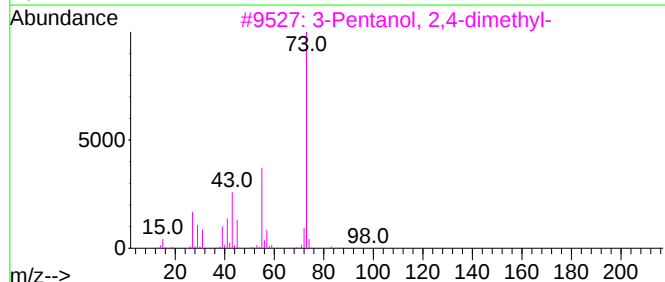
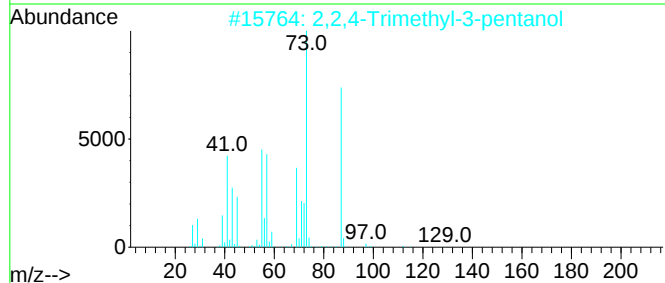
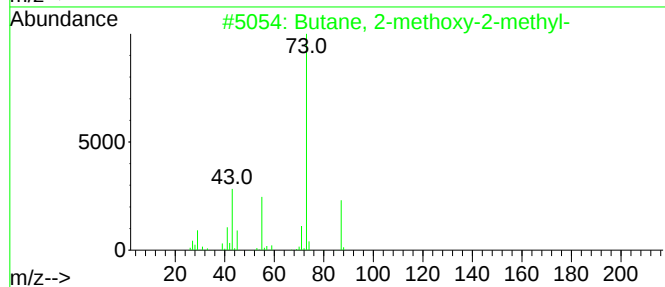
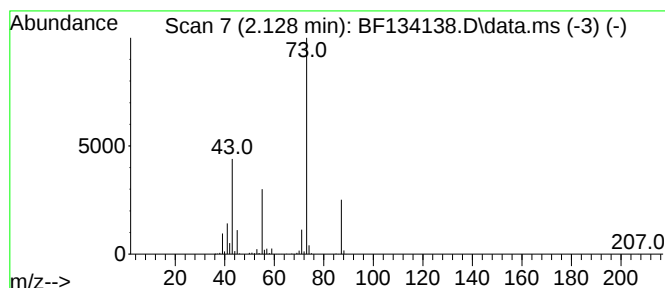
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	47.90 ng	1526180	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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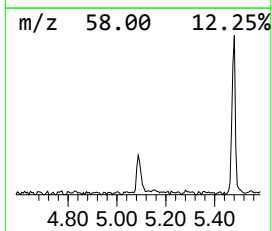
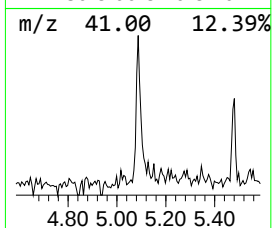
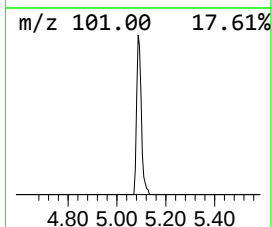
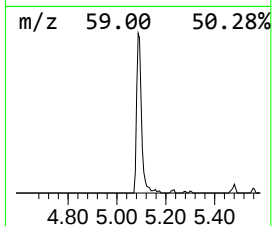
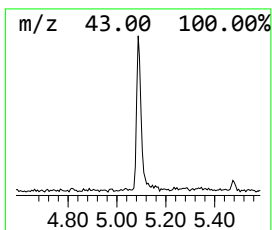
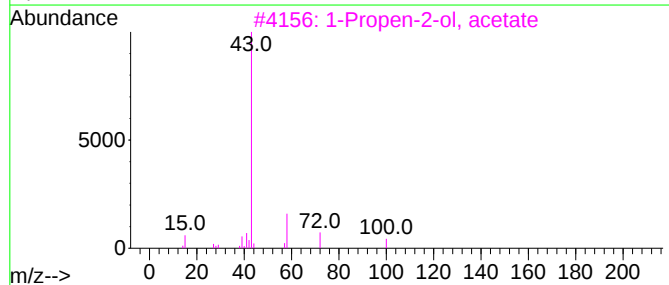
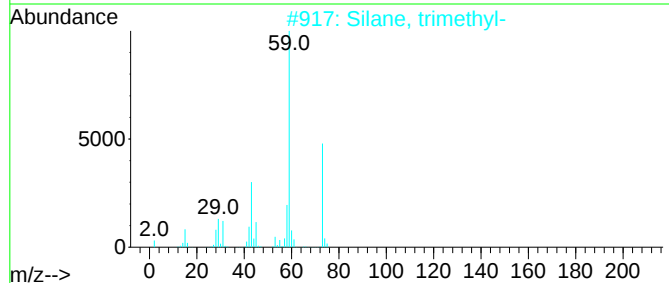
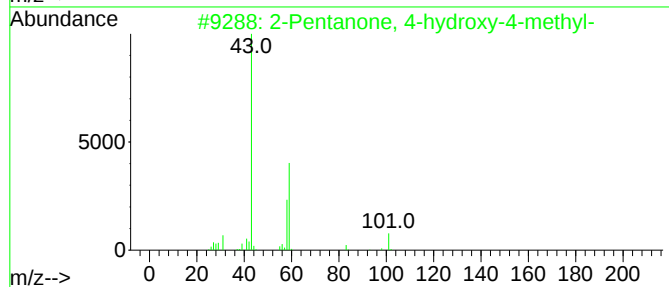
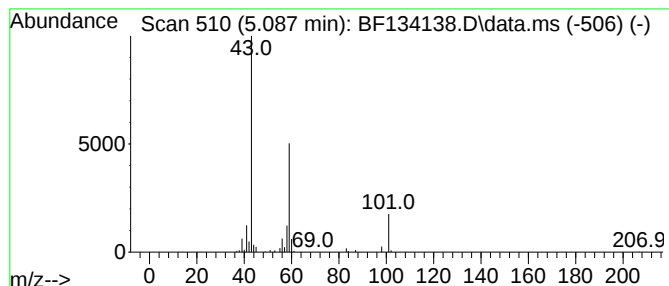
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.087 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	3.19 ng	101601	1,4-Dichlorobenzene-d4	6.845

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2		Silane, trimethyl-	74	C3H10Si	000993-07-7	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Butane	58	C4H10	000106-97-8	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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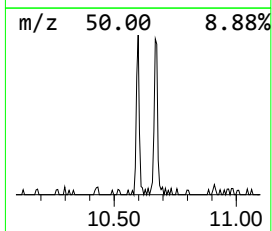
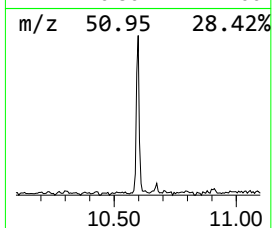
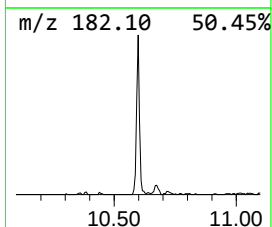
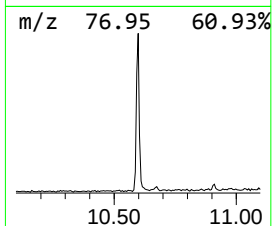
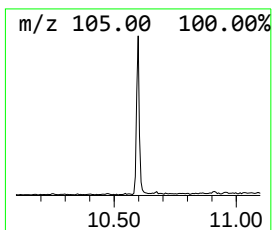
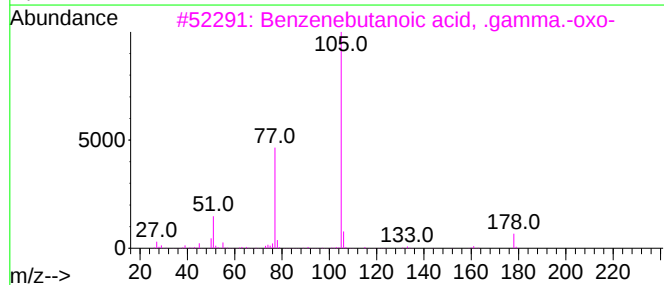
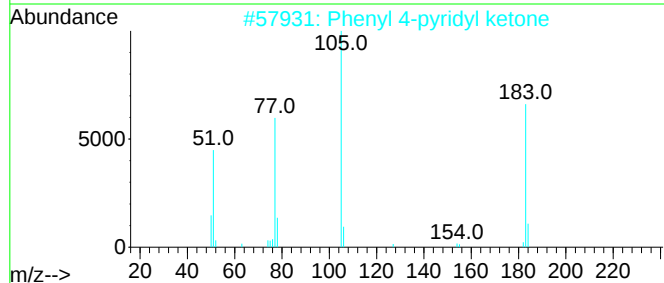
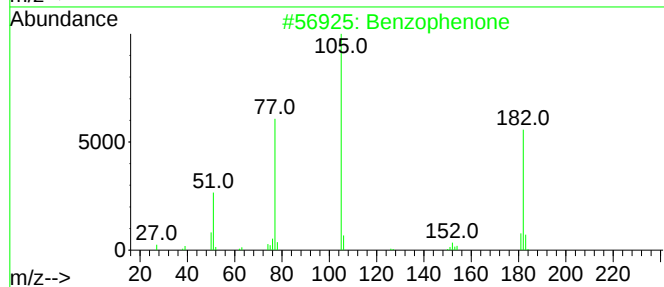
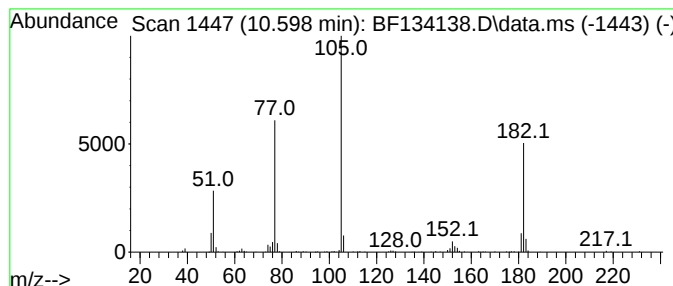
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	4.50 ng	169259	Acenaphthene-d10	9.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	49
4			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	49
5			Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	47



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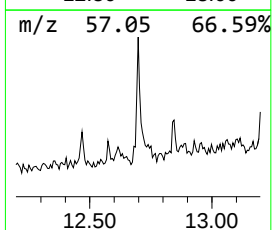
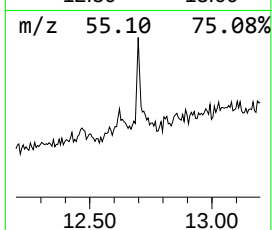
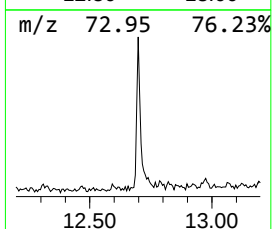
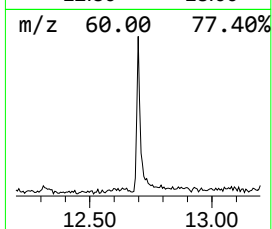
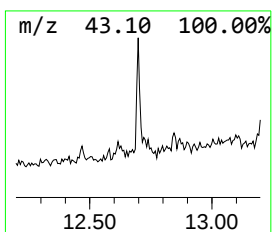
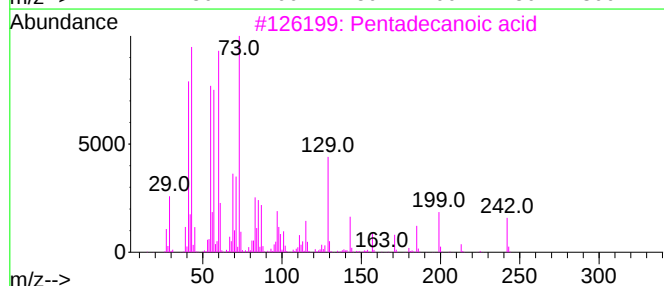
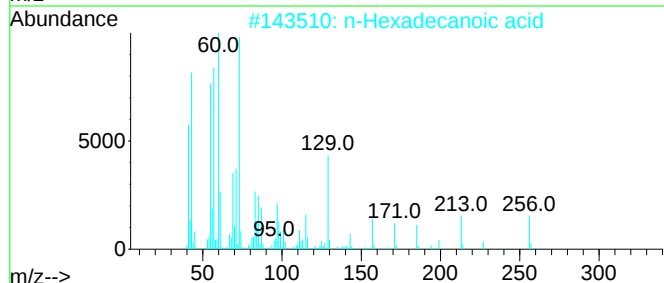
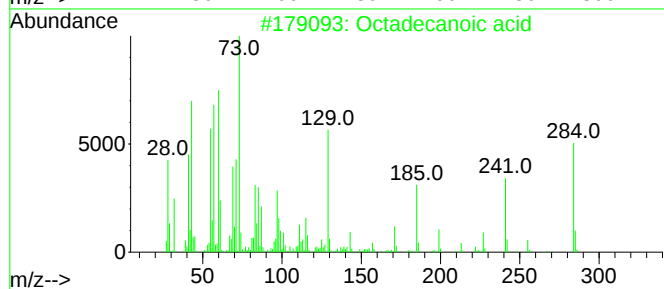
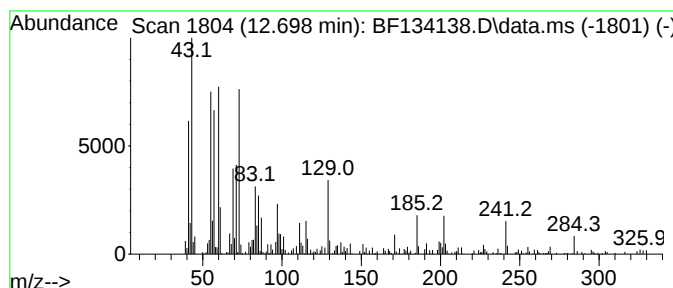
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.698	5.90 ng	186297	Phenanthrene-d10	11.374	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Heneicosanoic acid	326	C21H42O2	002363-71-5	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.128	47.9	ng	1526180	1	6.845	637238	20.0
unknown5.087	5.087	3.2	ng	101601	1	6.845	637238	20.0
Benzophenone	10.598	4.5	ng	169259	3	9.880	752188	20.0
Octadecanoic acid	12.698	5.9	ng	186297	4	11.374	631441	20.0