

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
 Data File : BF134107.D
 Acq On : 06 Jul 2023 20:41
 Operator : CG\JU
 Sample : 03476-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DOREMUS-COMP-1

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: BF134107.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	6	12	21	rVB	1251256	1720135	80.49%	9.032%
2	2.269	28	31	35	rVB	24102	29315	1.37%	0.154%
3	5.087	507	510	523	rVB	121812	159907	7.48%	0.840%
4	5.481	573	577	595	rBV	2318182	2112347	98.84%	11.091%
5	6.481	742	747	750	rBV	2242419	2106334	98.56%	11.060%
6	6.845	805	809	820	rBV	687623	559912	26.20%	2.940%
7	7.410	900	905	916	rBV	1366638	1361042	63.68%	7.146%
8	8.122	1023	1026	1044	rVB	822433	732136	34.26%	3.844%
9	9.204	1206	1210	1213	rBV	2492225	2137176	100.00%	11.222%
10	9.880	1322	1325	1329	rBV	934481	787883	36.87%	4.137%
11	10.598	1444	1447	1456	rBV	391448	329614	15.42%	1.731%
12	10.674	1456	1460	1470	rBV	1842564	1650177	77.21%	8.665%
13	10.910	1496	1500	1503	rBV	45659	39880	1.87%	0.209%
14	11.374	1575	1579	1582	rBV	944873	834007	39.02%	4.379%
15	11.398	1582	1583	1588	rVB	79881	54971	2.57%	0.289%
16	11.480	1595	1597	1601	rVB	33186	25059	1.17%	0.132%
17	11.904	1667	1669	1674	rBV2	219998	211480	9.90%	1.110%
18	11.992	1681	1684	1693	rVB2	20173	33803	1.58%	0.177%
19	12.598	1783	1787	1796	rBV	156045	153243	7.17%	0.805%
20	12.698	1801	1804	1811	rBV3	34432	46440	2.17%	0.244%
21	12.827	1821	1826	1831	rVB	124564	131190	6.14%	0.689%
22	12.974	1846	1851	1854	rBV	2441612	2111584	98.80%	11.087%
23	13.551	1945	1949	1953	rBV3	21685	26986	1.26%	0.142%
24	13.880	2002	2005	2007	rBV	31309	27624	1.29%	0.145%
25	13.921	2007	2012	2025	rVV6	64382	204622	9.57%	1.074%
26	14.033	2026	2031	2034	rVV	700437	725068	33.93%	3.807%
27	14.057	2034	2035	2043	rVB	63704	63270	2.96%	0.332%
28	14.198	2056	2059	2063	rBV2	27987	25666	1.20%	0.135%
29	14.504	2109	2111	2117	rBV4	26027	35984	1.68%	0.189%
30	15.098	2208	2212	2214	rBV2	33762	46156	2.16%	0.242%
31	15.409	2261	2265	2271	rVB	20162	27797	1.30%	0.146%
32	15.468	2272	2275	2281	rBV	26050	36720	1.72%	0.193%
33	15.539	2281	2287	2291	rBV	356944	497673	23.29%	2.613%

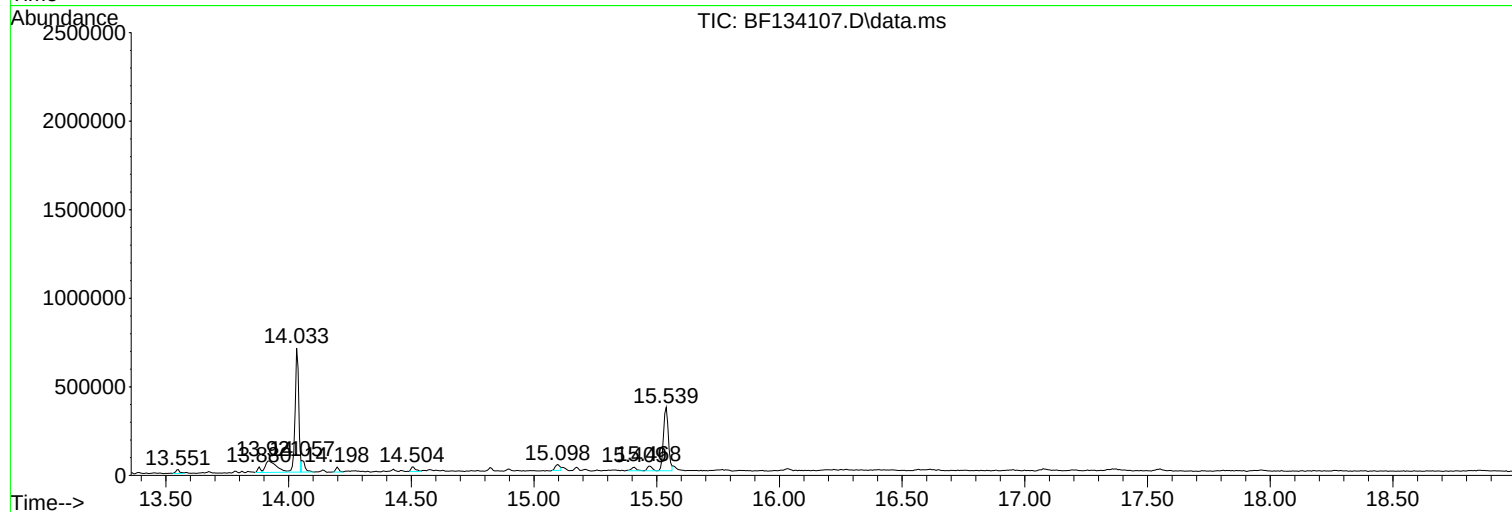
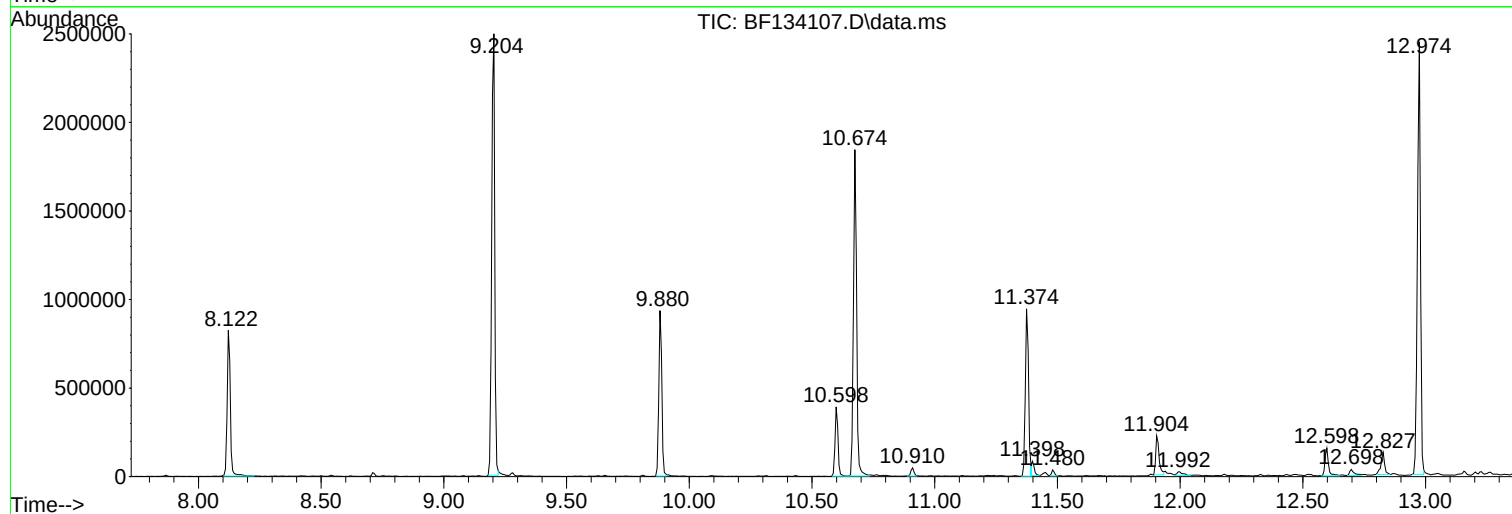
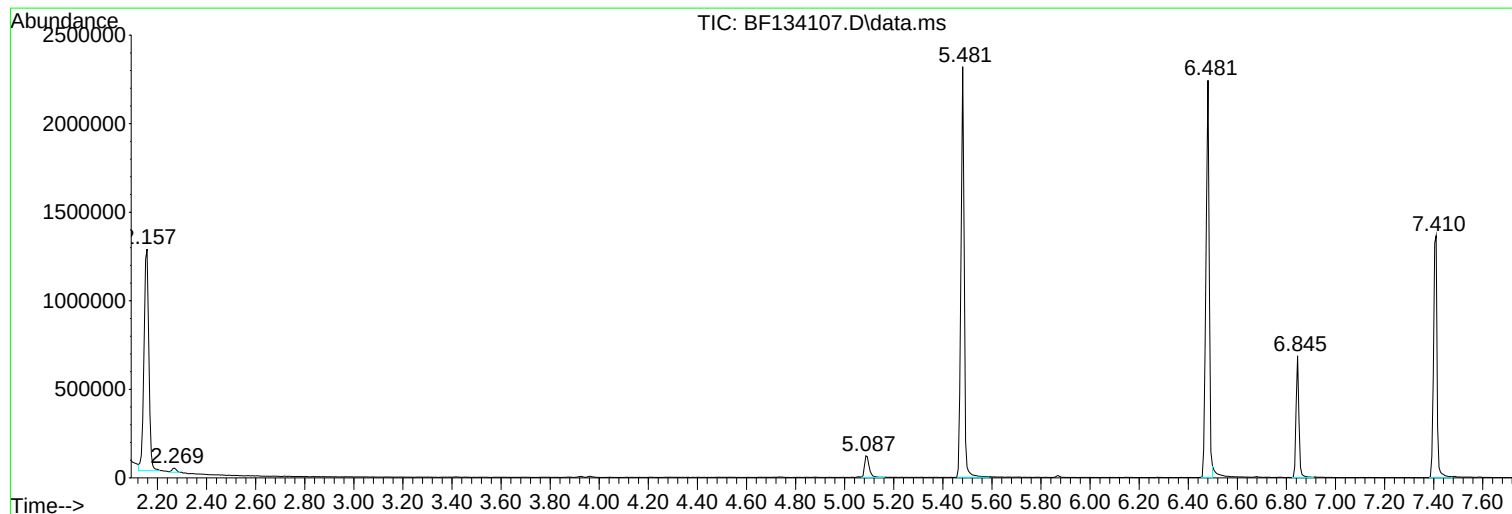
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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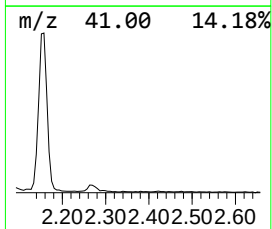
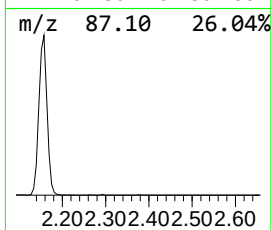
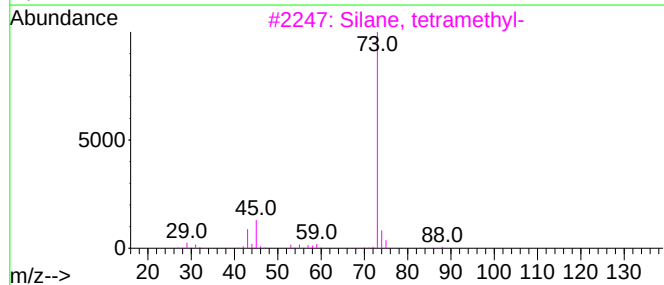
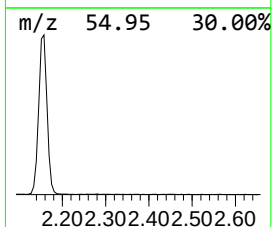
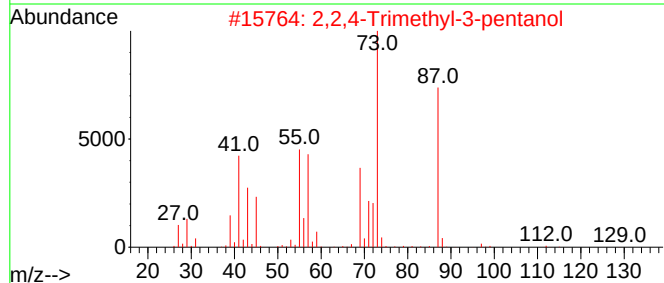
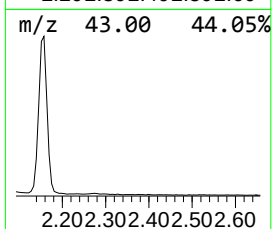
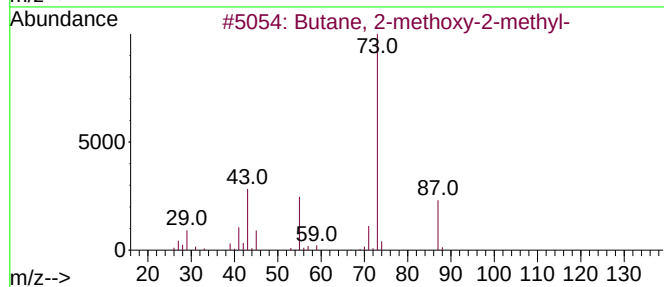
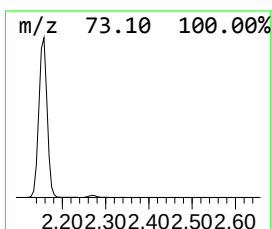
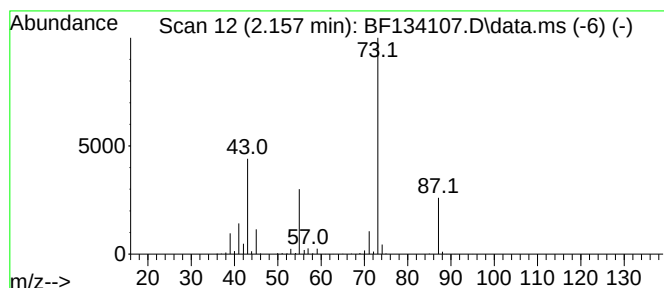
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.157	61.44 ng	1720140	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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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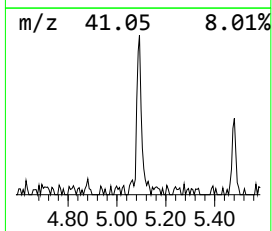
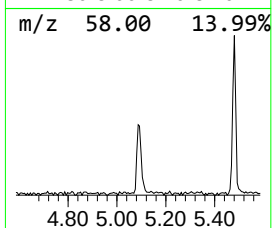
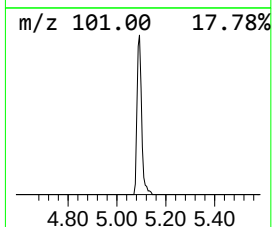
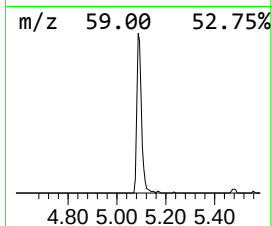
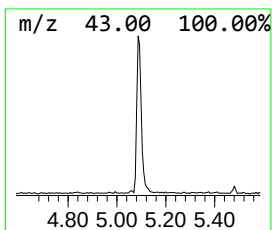
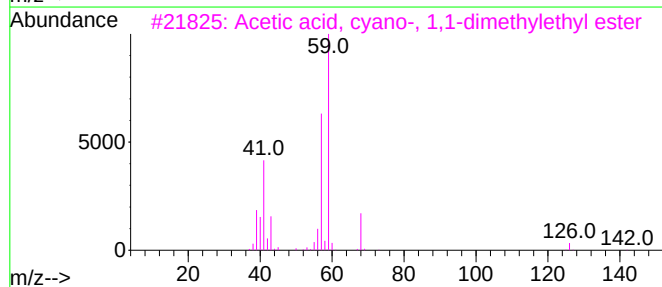
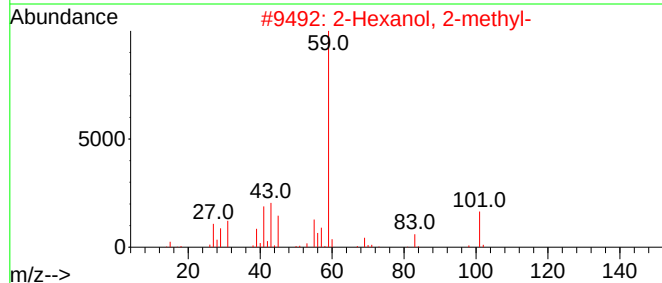
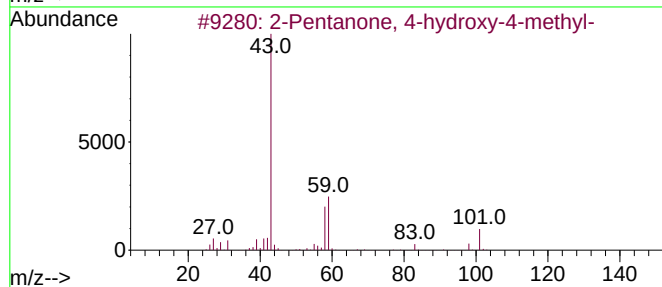
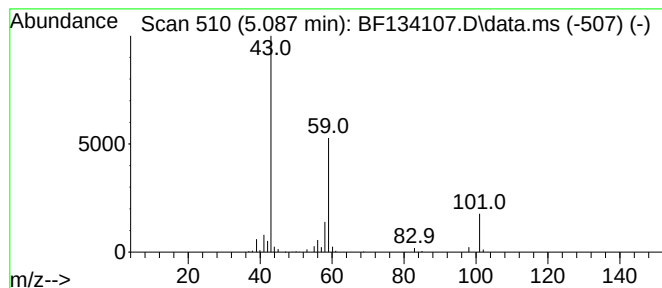
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	5.71 ng	159907	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	59		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		



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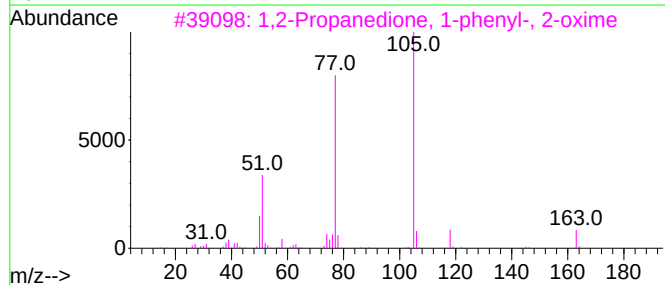
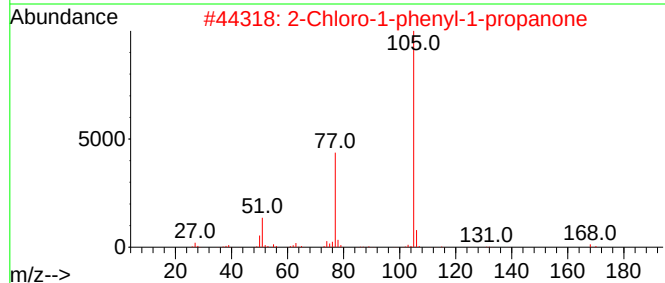
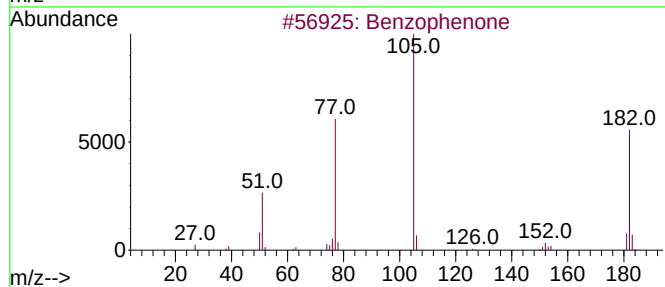
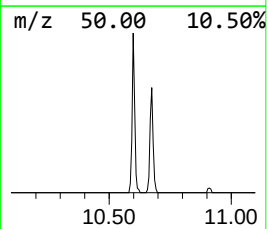
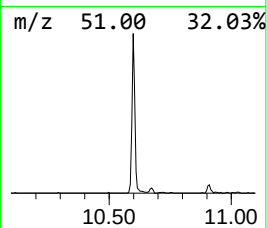
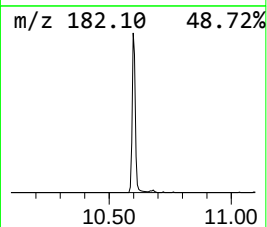
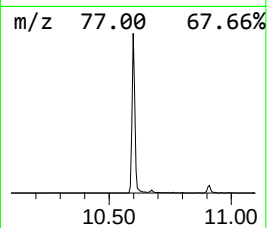
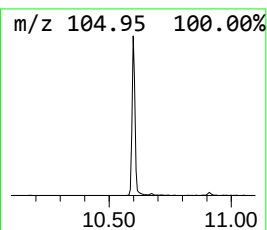
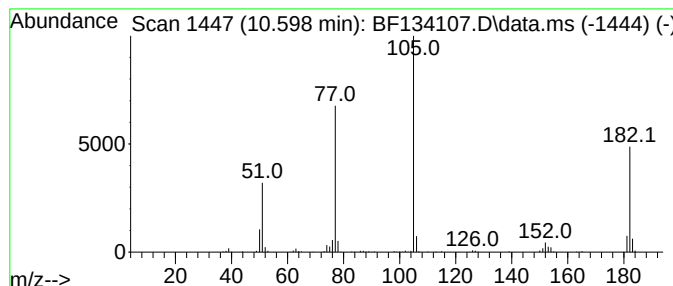
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	8.37 ng	329614	Acenaphthene-d10	9.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	50
3			1,2-Propanedione, 1-phenyl-, 2-o...	163	C9H9NO2	000119-51-7	50
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	50
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	50



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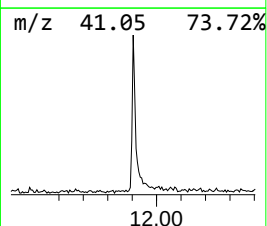
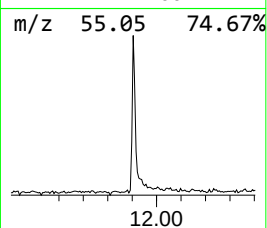
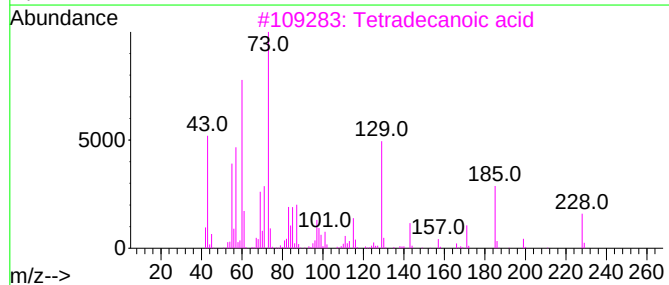
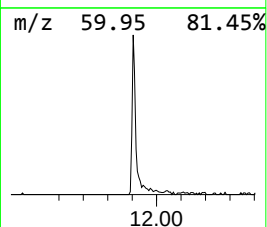
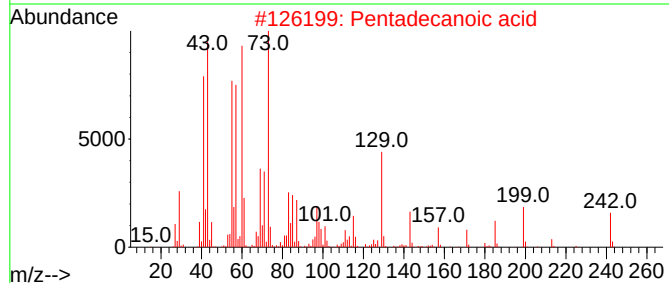
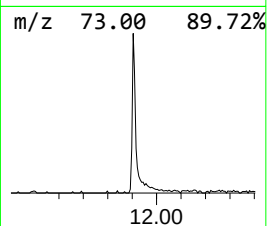
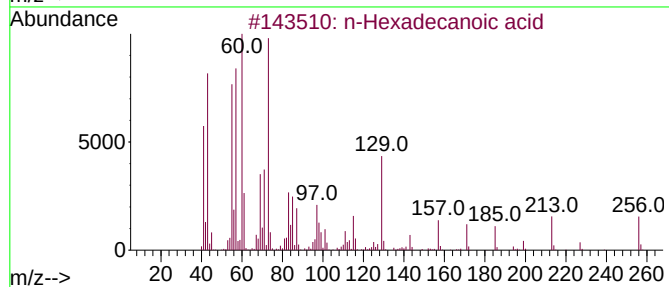
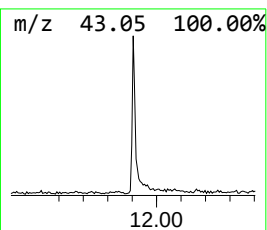
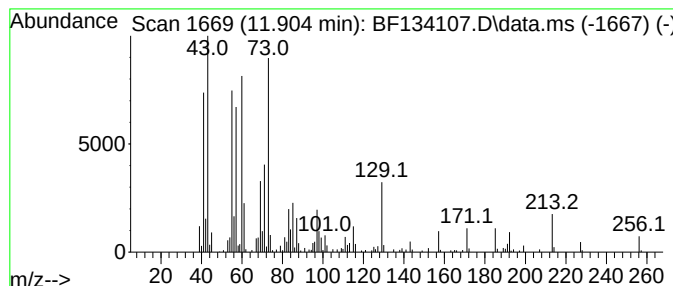
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	5.07 ng	211480	Phenanthrene-d10	11.374

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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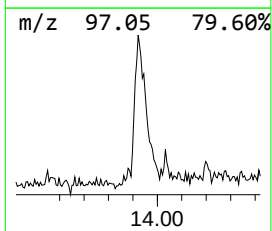
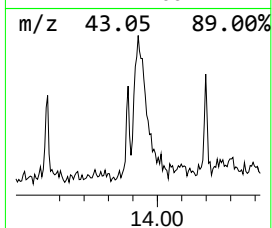
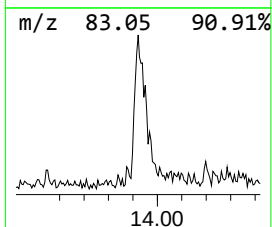
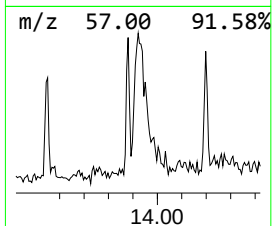
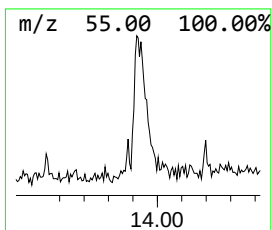
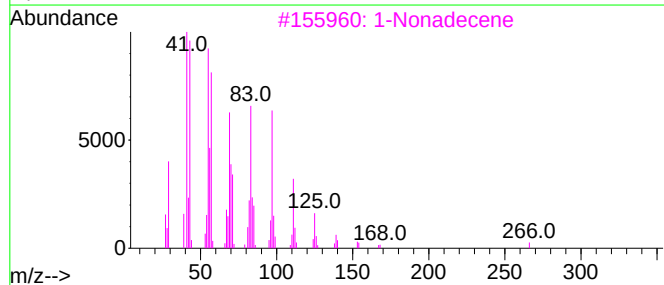
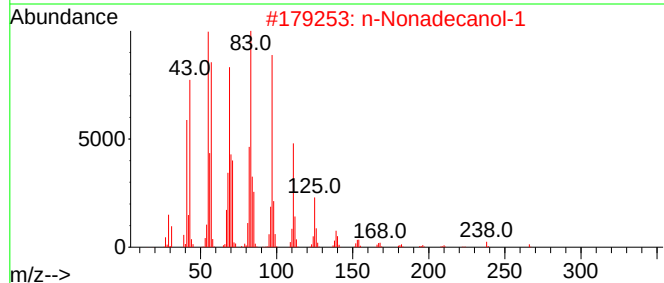
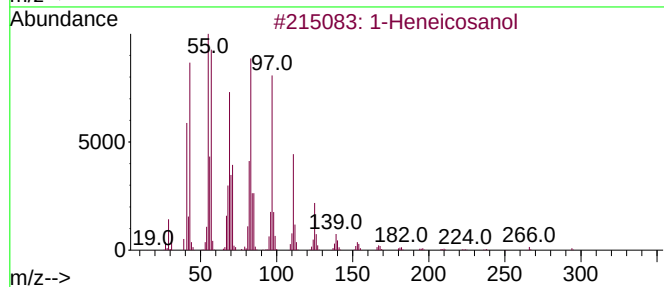
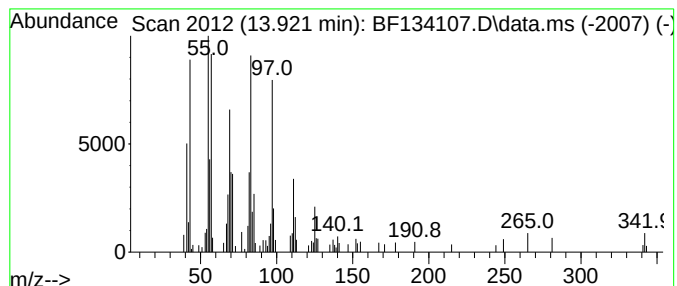
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	5.64 ng	204622	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		1-Octadecanol	270	C18H38O	000112-92-5	83
5		Behenic alcohol	326	C22H46O	000661-19-8	83



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.157	61.4	ng	1720140	1	6.845	559912	20.0
2-Pentanone, 4-...	5.087	5.7	ng	159907	1	6.845	559912	20.0
Benzophenone	10.598	8.4	ng	329614	3	9.880	787883	20.0
n-Hexadecanoic ...	11.904	5.1	ng	211480	4	11.374	834007	20.0
1-Heneicosanol	13.921	5.6	ng	204622	5	14.033	725068	20.0