

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
 Data File : BF140119.D
 Acq On : 29 Oct 2024 18:37
 Operator : RC/JU
 Sample : P4597-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BLUE-2-1

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140119.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	11	18	29	rVB	969522	1535216	51.25%	6.417%
2	5.116	506	514	521	rVB	159154	252063	8.41%	1.054%
3	5.504	574	580	586	rBV	1710993	2342831	78.21%	9.792%
4	6.504	744	750	756	rBV	1745256	2443341	81.57%	10.213%
5	6.887	810	815	820	rBV	660963	801098	26.74%	3.348%
6	7.446	903	910	915	rBV	1267532	1680784	56.11%	7.025%
7	7.698	949	953	960	rVB	37845	47532	1.59%	0.199%
8	8.169	1027	1033	1038	rBV	844783	1083211	36.16%	4.528%
9	9.245	1209	1216	1226	rBV	2183085	2995427	100.00%	12.520%
10	9.922	1326	1331	1346	rVB	992615	1267265	42.31%	5.297%
11	10.634	1448	1452	1459	rBV	529968	684169	22.84%	2.860%
12	10.710	1460	1465	1479	rBV	1380539	1802485	60.17%	7.534%
13	10.945	1497	1505	1514	rBV	82363	103798	3.47%	0.434%
14	11.410	1579	1584	1592	rBV	999101	1358521	45.35%	5.678%
15	11.933	1664	1673	1685	rBV3	190696	324058	10.82%	1.354%
16	12.028	1685	1689	1697	rVB3	17058	36398	1.22%	0.152%
17	12.622	1785	1790	1796	rBV	165036	209877	7.01%	0.877%
18	12.716	1802	1806	1814	rBV4	23837	45496	1.52%	0.190%
19	12.851	1822	1829	1834	rBV	126781	180194	6.02%	0.753%
20	12.998	1846	1854	1859	rBV	1879182	2425771	80.98%	10.139%
21	13.904	2003	2008	2026	rBV3	65682	177896	5.94%	0.744%
22	14.063	2027	2035	2047	rVB	585509	906681	30.27%	3.790%
23	15.139	2212	2218	2228	rBV	66603	155900	5.20%	0.652%
24	15.221	2228	2232	2240	rVV2	24393	39894	1.33%	0.167%
25	15.445	2265	2270	2276	rVB	34658	52761	1.76%	0.221%
26	15.510	2276	2281	2286	rBV	34803	54152	1.81%	0.226%
27	15.580	2286	2293	2308	rVB	445061	768603	25.66%	3.213%
28	16.063	2370	2375	2382	rVB	30270	56256	1.88%	0.235%
29	17.080	2542	2548	2560	rBV2	19118	53632	1.79%	0.224%
30	17.527	2619	2624	2635	rVB	16804	39643	1.32%	0.166%

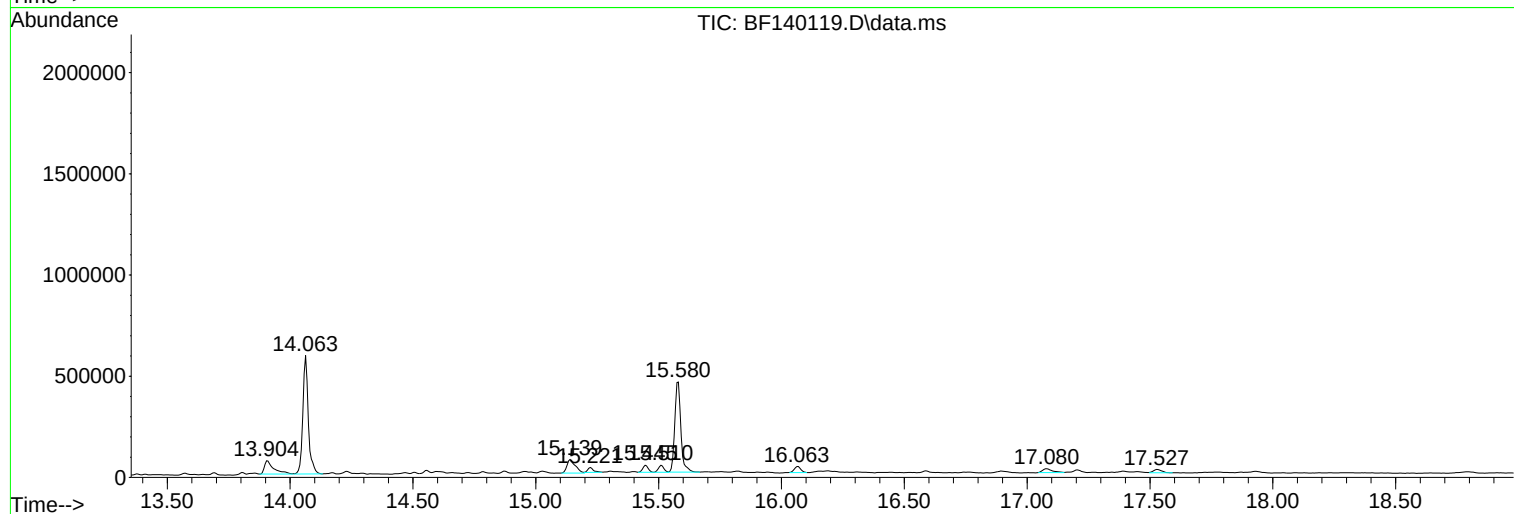
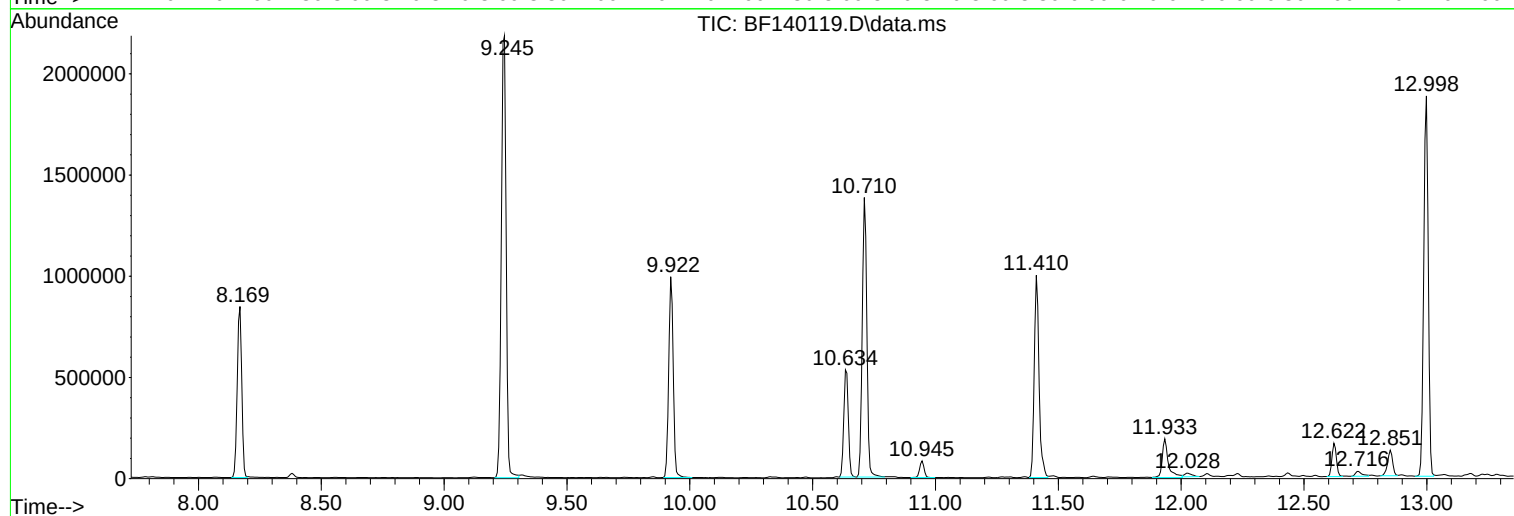
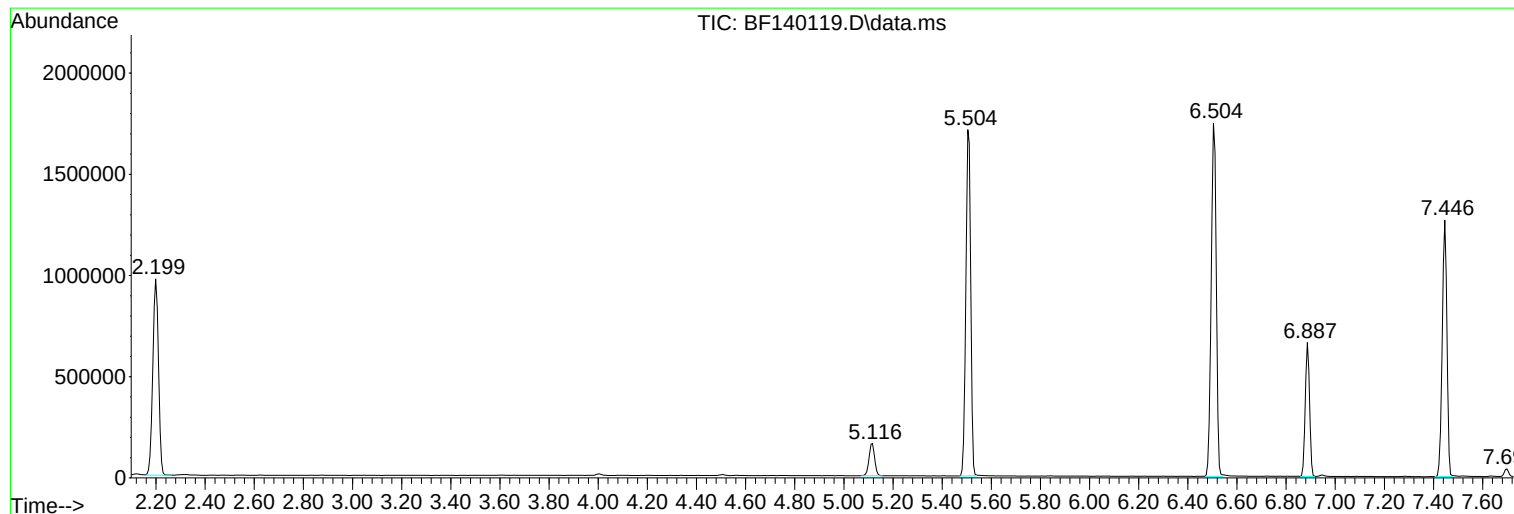
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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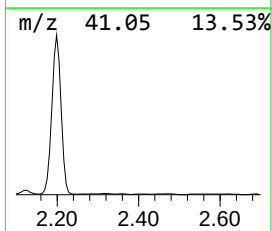
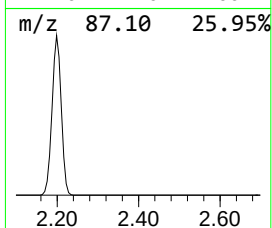
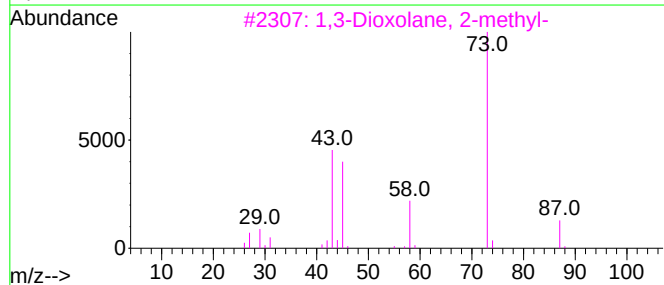
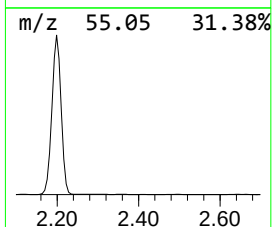
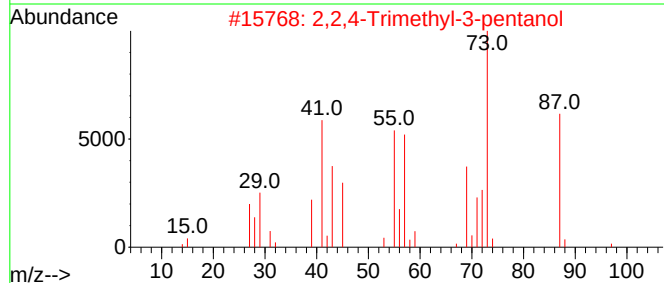
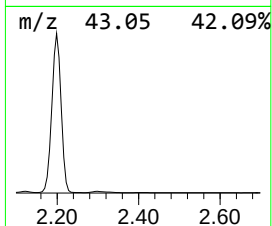
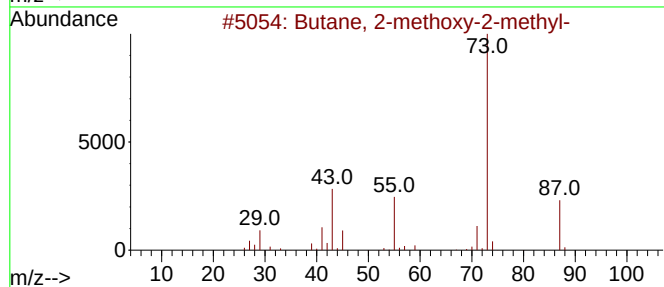
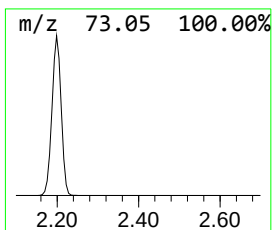
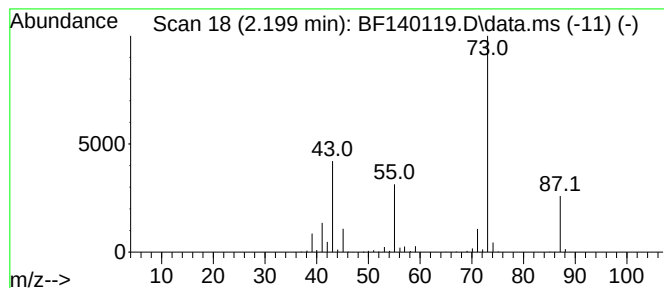
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	38.33 ng	1535220	1,4-Dichlorobenzene-d4	6.887

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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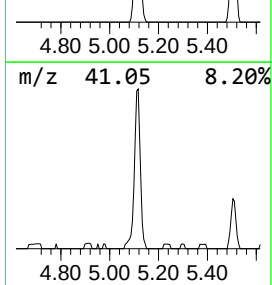
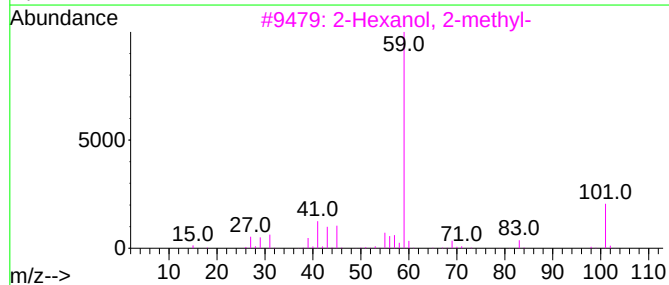
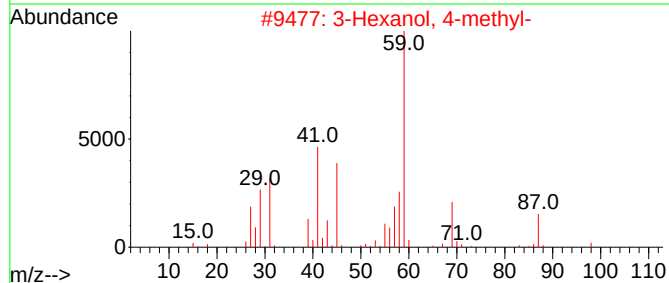
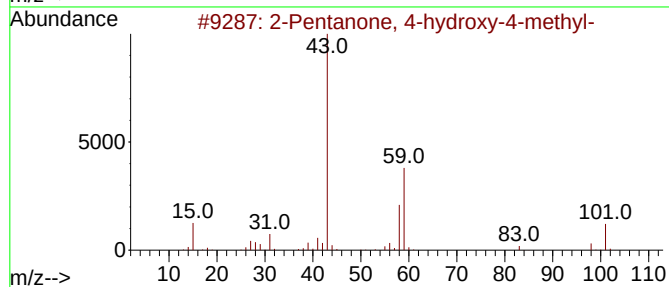
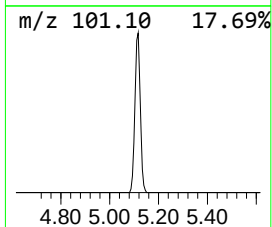
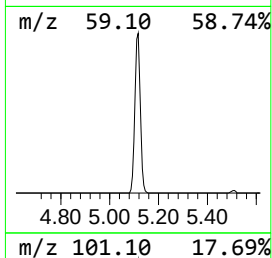
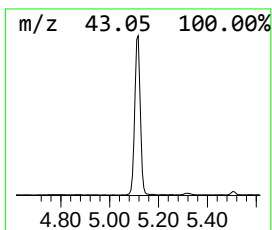
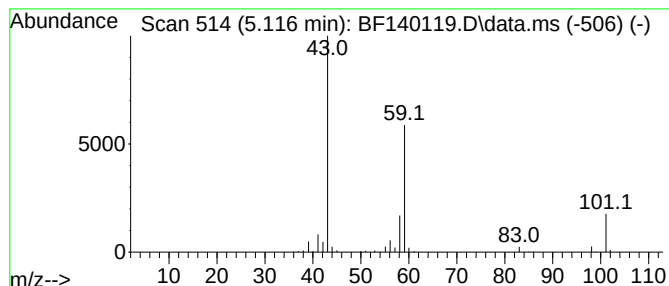
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.116	6.29 ng	252063	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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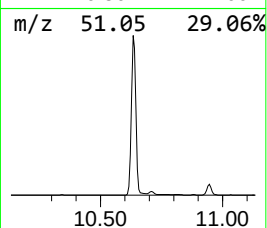
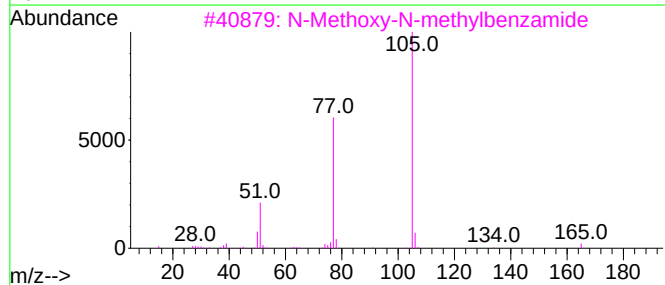
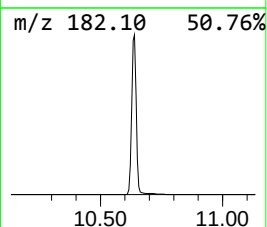
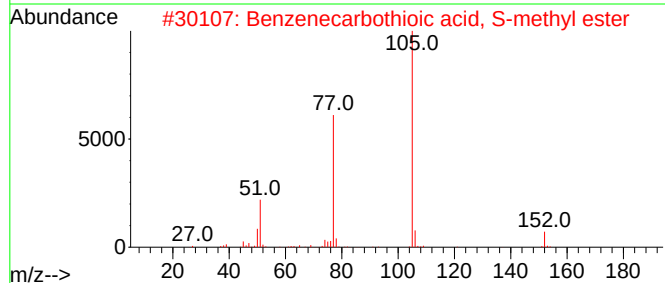
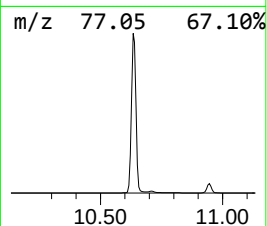
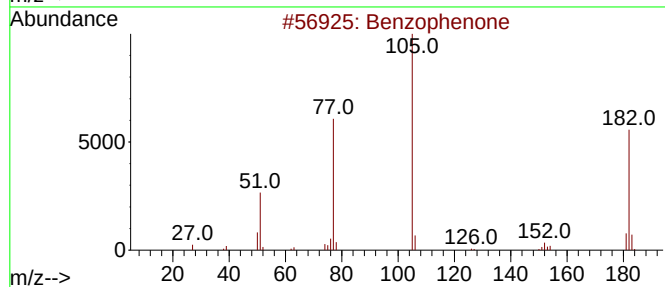
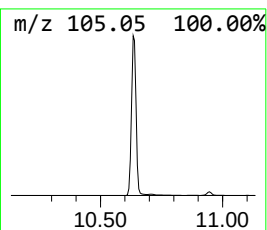
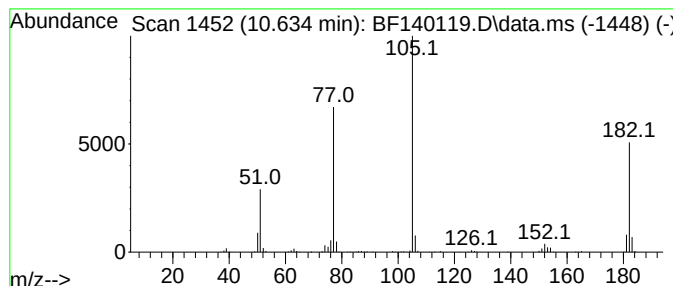
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	10.80 ng	684169	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	47
5			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47



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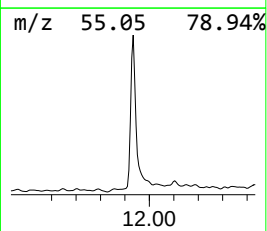
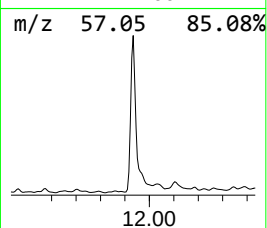
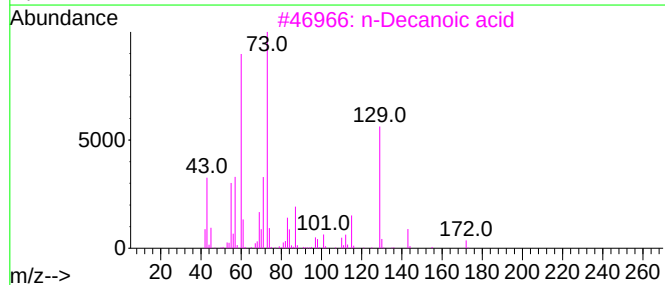
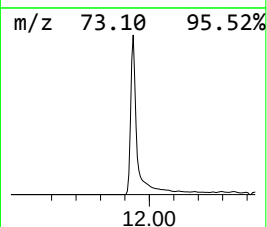
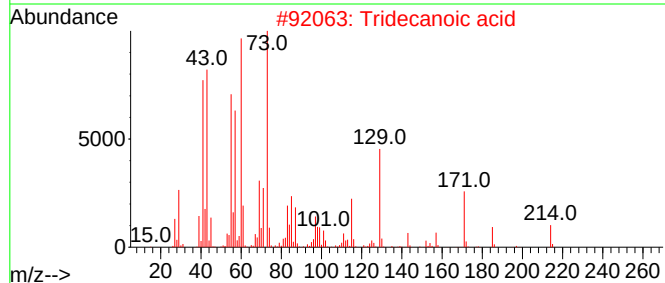
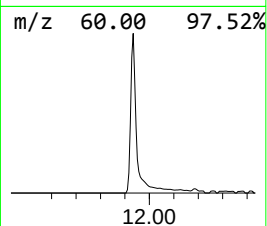
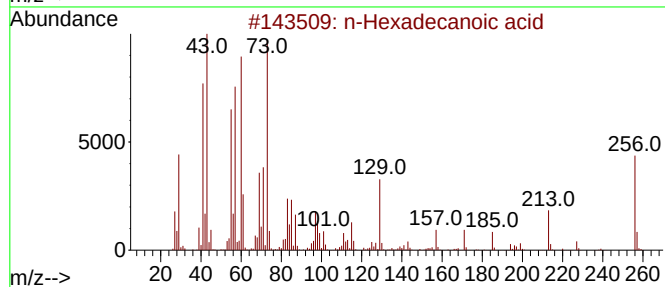
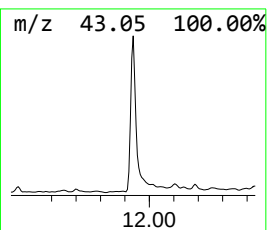
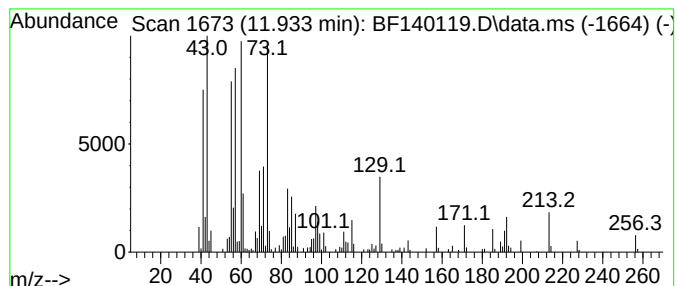
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.934	4.77 ng	324058	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			n-Decanoic acid	172	C10H20O2	000334-48-5	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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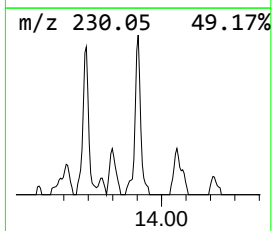
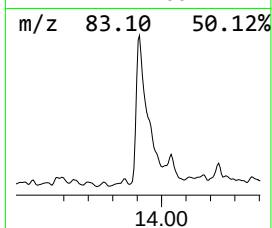
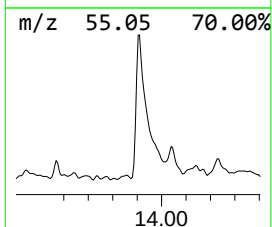
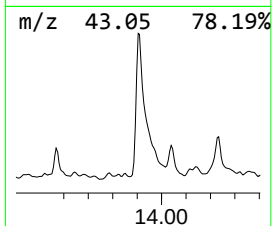
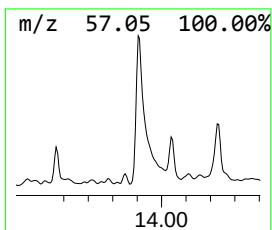
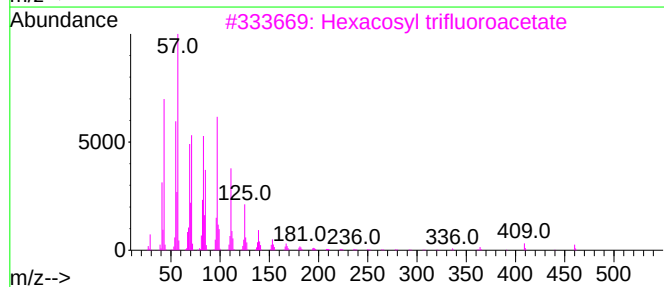
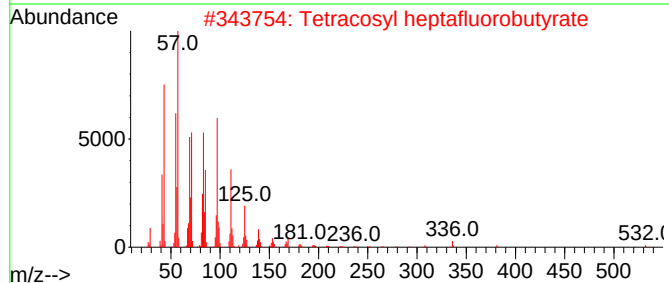
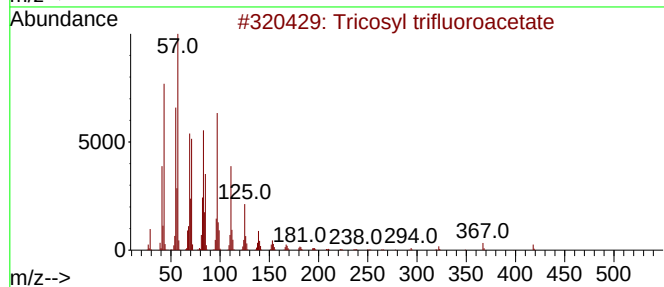
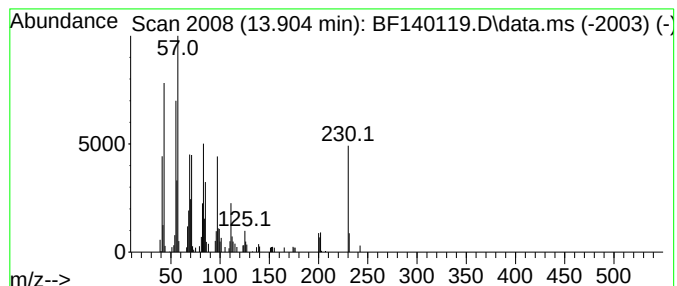
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tricosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.92 ng	177896	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	81
2			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	81
3			Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	81
4			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	81
5			Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	81



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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...	2.199	38.3	ng	1535220	1	6.887	801098	20.0
2-Pentanone, 4-...	5.116	6.3	ng	252063	1	6.887	801098	20.0
Benzophenone	10.634	10.8	ng	684169	3	9.922	1267270	20.0
n-Hexadecanoic ...	11.934	4.8	ng	324058	4	11.410	1358520	20.0
Tricosyl triflu...	13.904	3.9	ng	177896	5	14.063	906681	20.0