

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
 Data File : BF140116.D
 Acq On : 29 Oct 2024 17:18
 Operator : RC/JU
 Sample : P4594-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BP-F17

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: BF140116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	11	19	29	rVB	1199271	1931415	57.14%	7.281%
2	5.122	506	515	527	rVB2	22507	41674	1.23%	0.157%
3	5.510	574	581	586	rBV	1989889	2759478	81.64%	10.402%
4	6.510	744	751	756	rBV	1941854	2884077	85.33%	10.872%
5	6.887	810	815	820	rBV	657442	802891	23.75%	3.027%
6	7.445	903	910	915	rBV	1427424	1925148	56.96%	7.257%
7	7.698	948	953	960	rVB	56752	71712	2.12%	0.270%
8	8.169	1026	1033	1038	rBV	829666	1081368	31.99%	4.076%
9	8.381	1063	1069	1077	rVB	27636	36585	1.08%	0.138%
10	9.245	1209	1216	1221	rBV	2508110	3379905	100.00%	12.741%
11	9.322	1225	1229	1238	rVB	25354	41142	1.22%	0.155%
12	9.851	1312	1319	1323	rBV	34526	44607	1.32%	0.168%
13	9.922	1323	1331	1346	rVB	981273	1278714	37.83%	4.820%
14	10.351	1397	1404	1408	rBV	42509	59320	1.76%	0.224%
15	10.639	1447	1453	1459	rVV	435117	581004	17.19%	2.190%
16	10.710	1459	1465	1480	rVV	1628114	2288410	67.71%	8.627%
17	10.827	1480	1485	1494	rVB2	52928	91722	2.71%	0.346%
18	10.945	1500	1505	1513	rVB	64587	83067	2.46%	0.313%
19	11.274	1556	1561	1564	rBV	40519	54236	1.60%	0.204%
20	11.410	1579	1584	1589	rBV	1023369	1287799	38.10%	4.855%
21	11.474	1591	1595	1600	rVB2	32301	43814	1.30%	0.165%
22	11.698	1629	1633	1638	rBV	34402	42224	1.25%	0.159%
23	11.933	1668	1673	1697	rBV	363871	618926	18.31%	2.333%
24	12.104	1698	1702	1708	rVV2	43304	60380	1.79%	0.228%
25	12.721	1802	1807	1820	rBV	72763	139645	4.13%	0.526%
26	12.998	1848	1854	1859	rBV	2438119	3181338	94.13%	11.993%
27	13.904	2002	2008	2028	rBV2	53564	173389	5.13%	0.654%
28	14.057	2028	2034	2045	rVB	601206	803047	23.76%	3.027%
29	15.557	2283	2289	2304	rVB	433601	740107	21.90%	2.790%

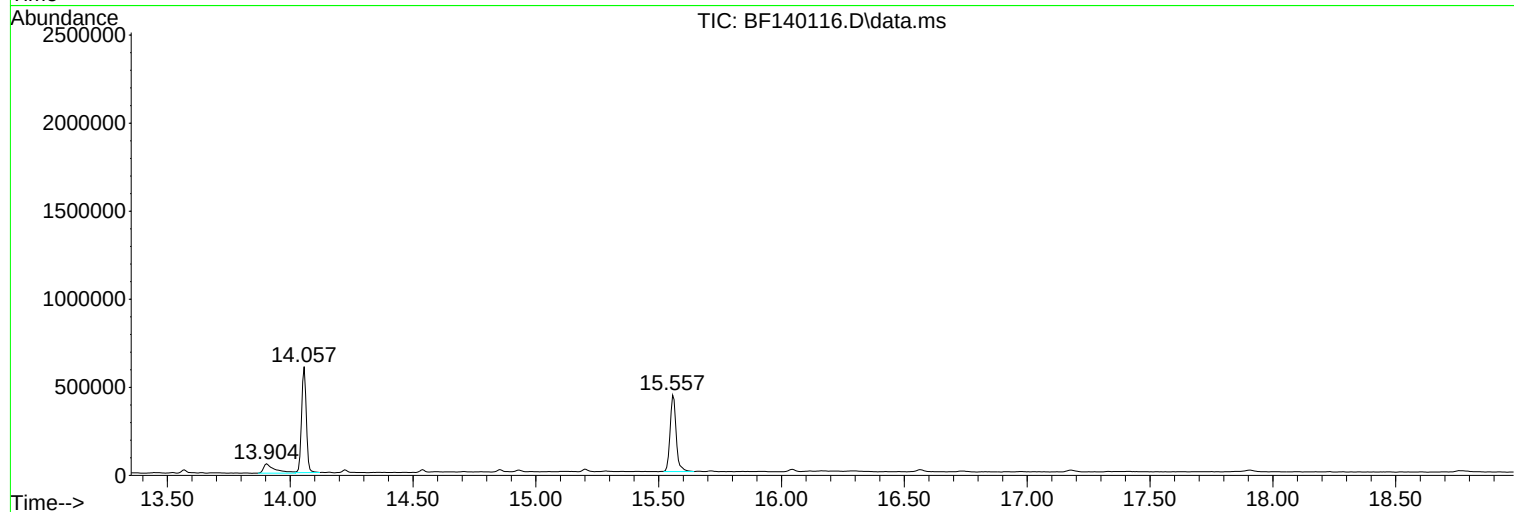
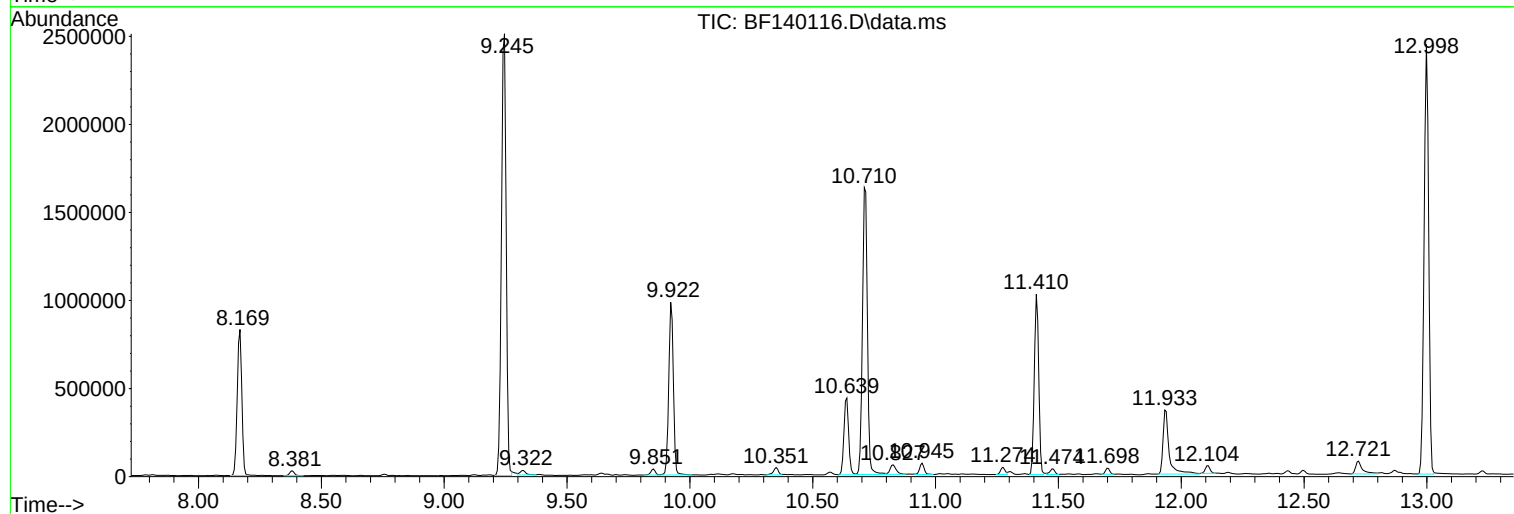
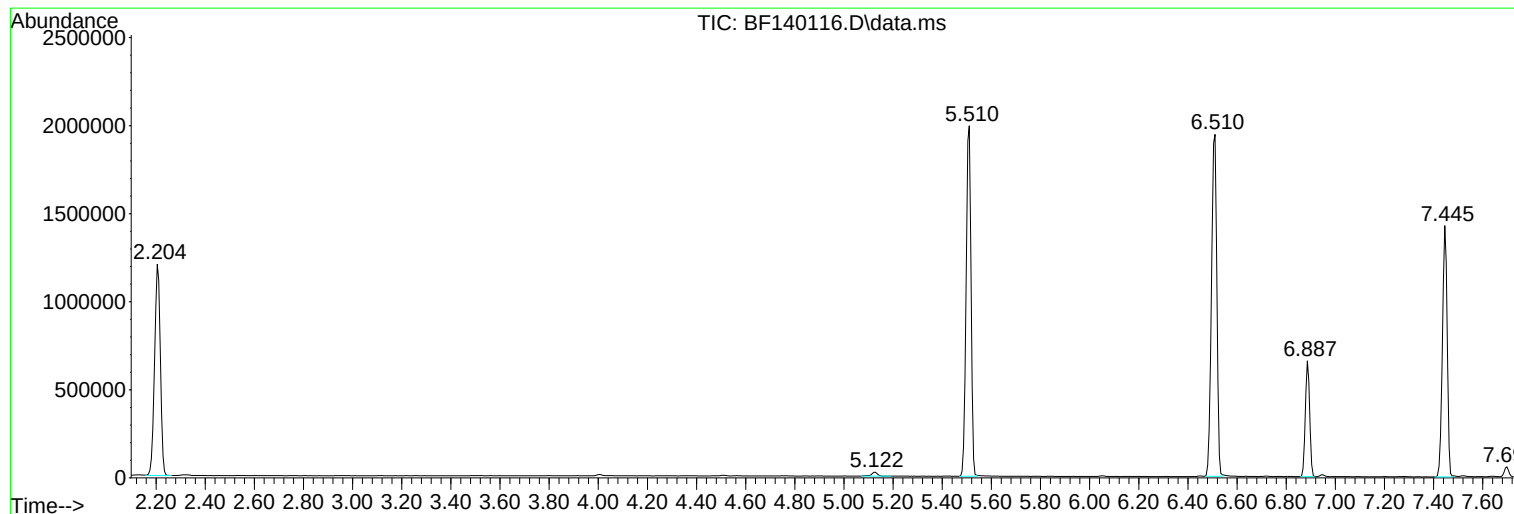
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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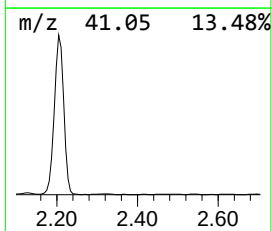
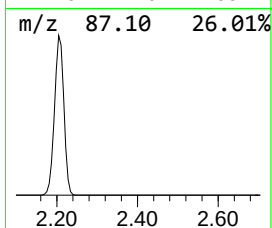
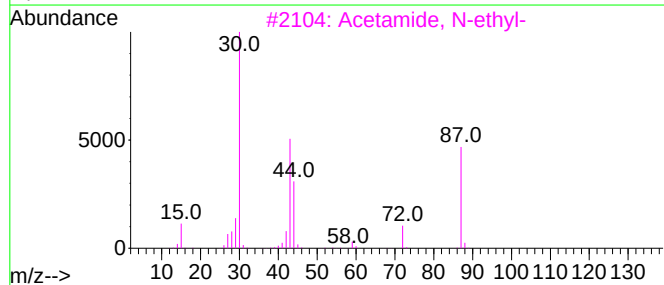
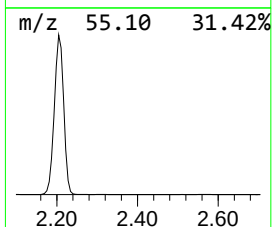
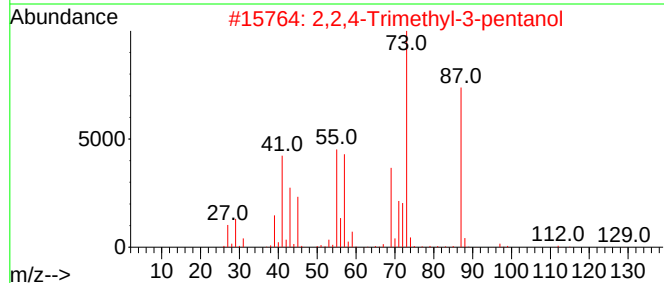
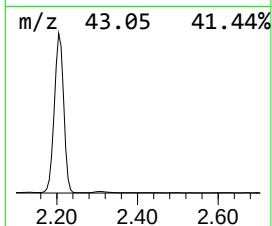
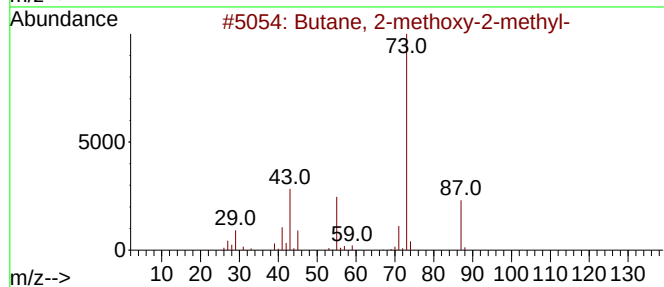
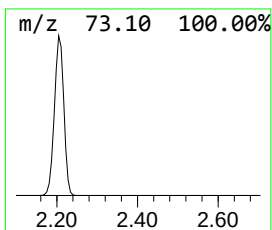
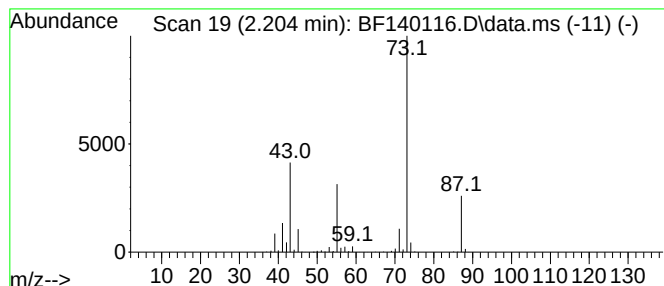
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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.
2.204	48.11 ng	1931420	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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17



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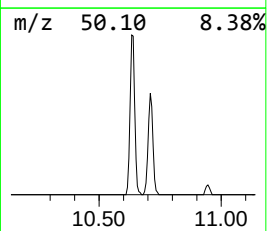
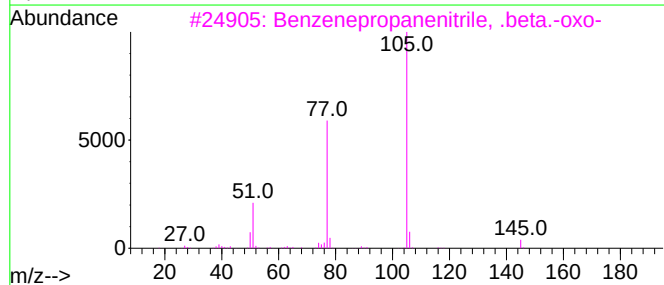
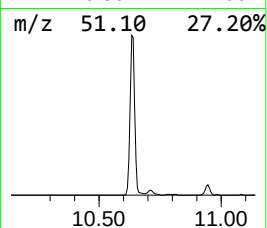
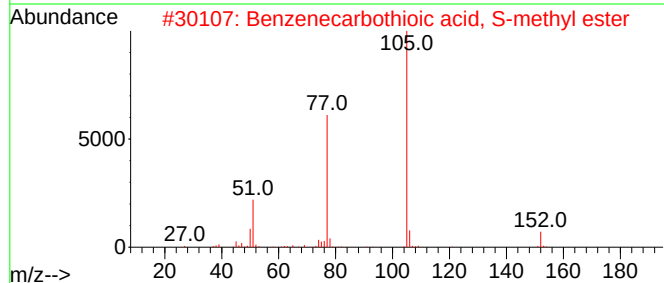
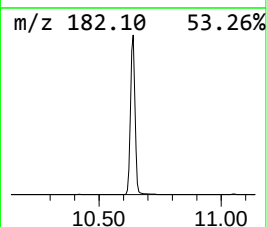
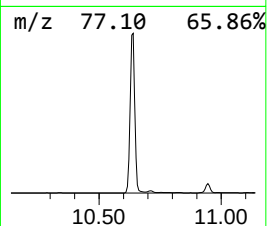
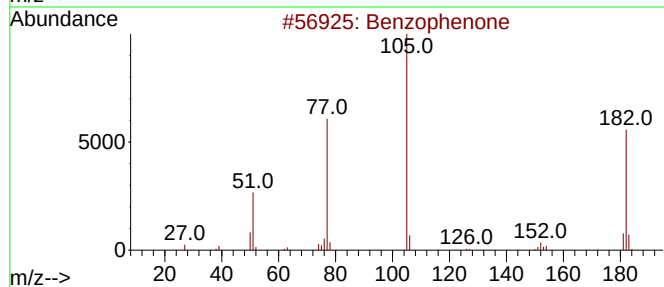
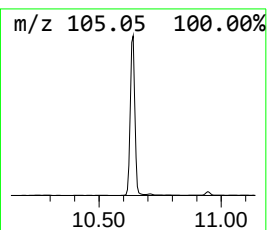
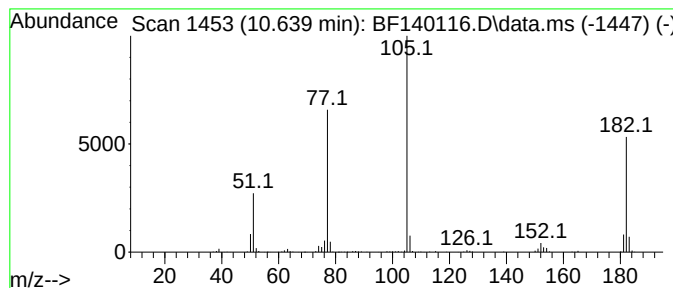
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	9.09 ng	581004	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	58
3			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
4			Vinyl benzoate	148	C9H8O2	000769-78-8	47
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



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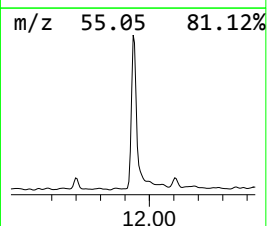
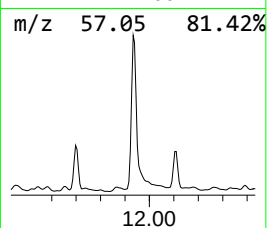
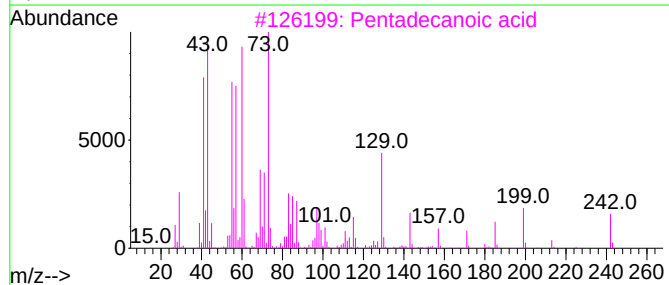
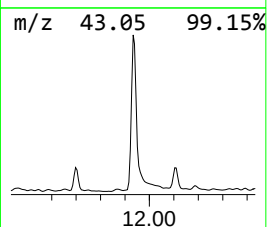
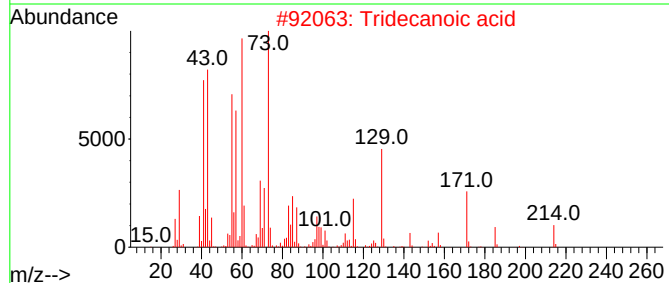
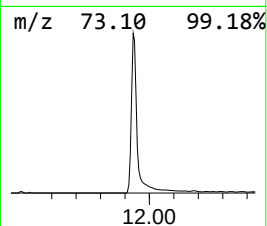
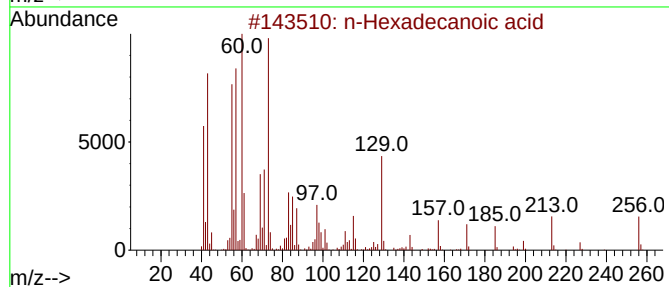
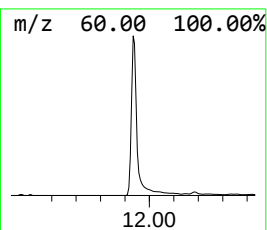
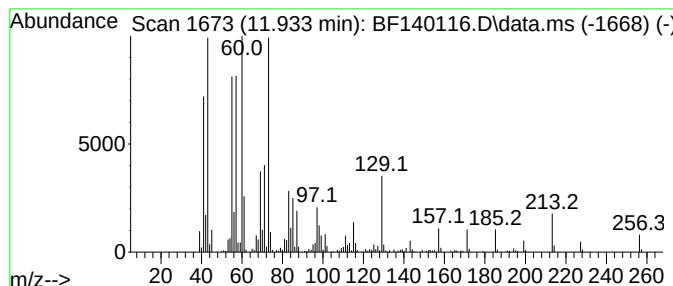
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	9.61 ng	618926	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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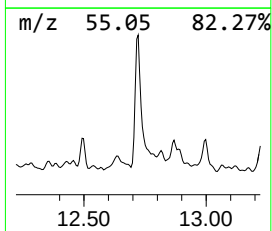
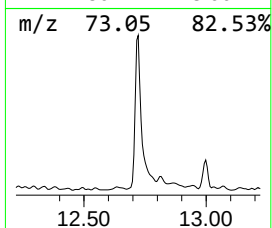
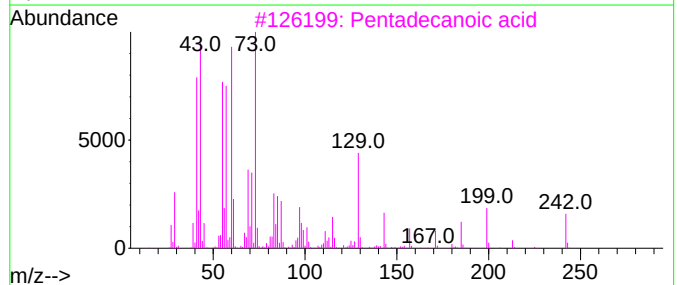
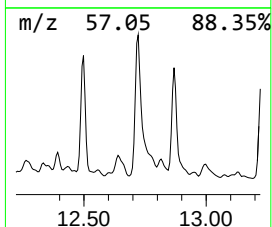
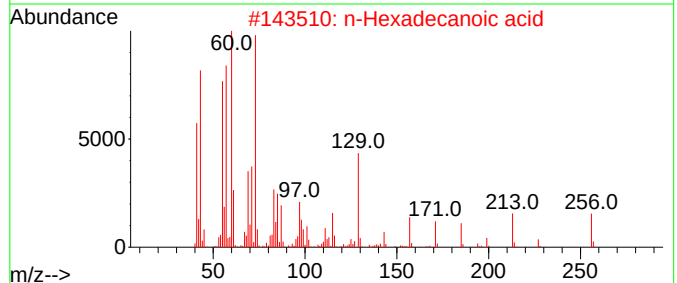
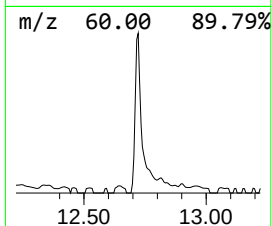
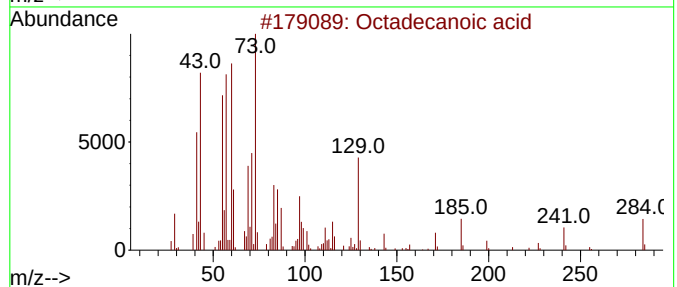
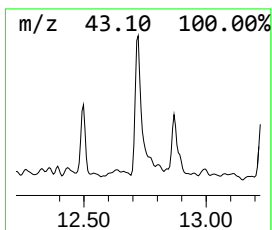
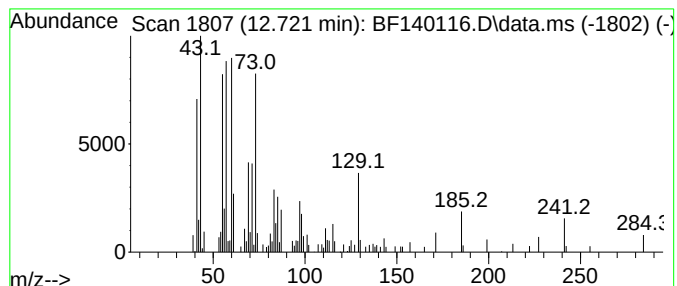
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.721	2.17 ng	139645	Phenanthrene-d10	11.410

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	91
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Undecanoic acid	186	C11H22O2	000112-37-8	83
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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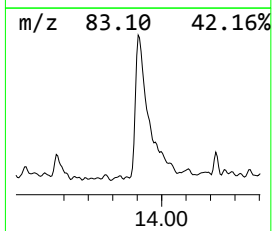
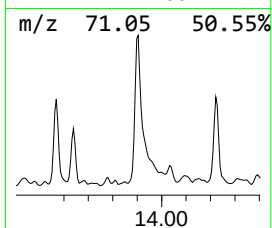
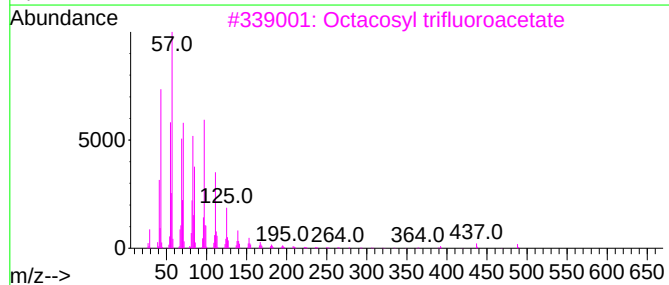
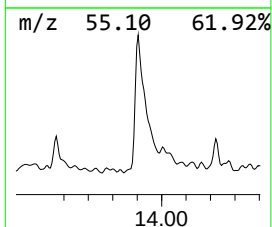
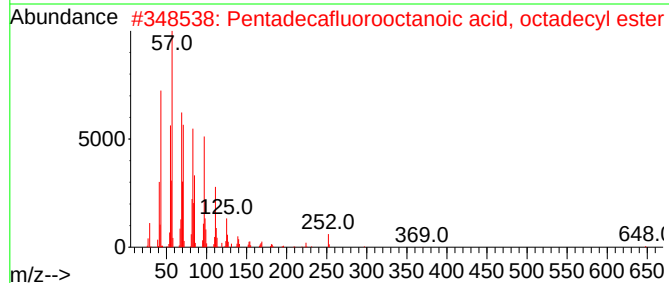
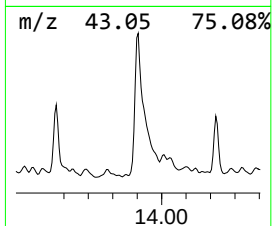
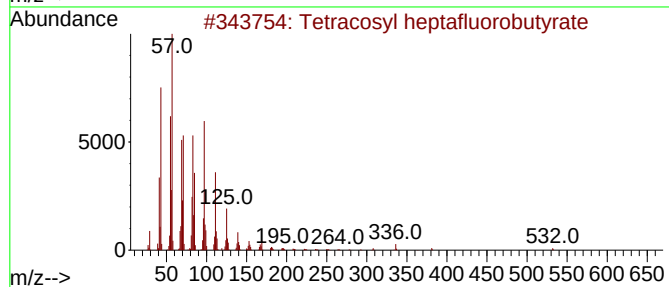
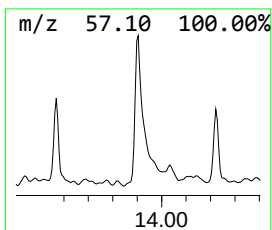
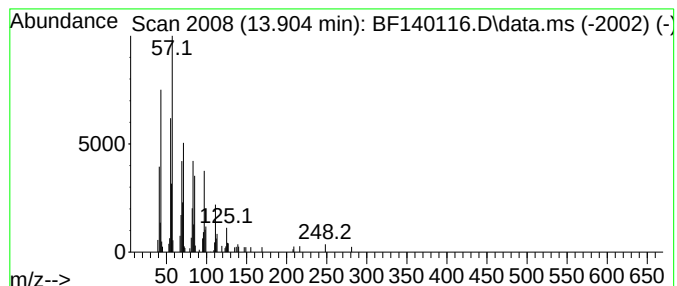
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tetracosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.32 ng	173389	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4			Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	91
5			Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.204	48.1	ng	1931420	1	6.887	802891	20.0
Benzophenone	10.639	9.1	ng	581004	3	9.922	1278710	20.0
n-Hexadecanoic ...	11.933	9.6	ng	618926	4	11.410	1287800	20.0
Octadecanoic acid	12.721	2.2	ng	139645	4	11.410	1287800	20.0
Tetracosyl hept...	13.904	4.3	ng	173389	5	14.057	803047	20.0