

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121024\
 Data File : BF140817.D
 Acq On : 10 Dec 2024 20:11
 Operator : RC/JU
 Sample : P5216-05
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-743

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-BF112124.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140817.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	9	24	rVB	1204677	2004413	100.00%	15.960%
2	5.510	576	581	601	rBV	854927	1172673	58.50%	9.337%
3	6.516	747	752	766	rBV	875059	1173580	58.55%	9.345%
4	6.863	806	811	816	rBV	297712	373685	18.64%	2.975%
5	7.428	901	907	912	rBV	596239	774264	38.63%	6.165%
6	7.681	946	950	956	rBV	27306	35018	1.75%	0.279%
7	8.139	1024	1028	1035	rBV	346669	469883	23.44%	3.741%
8	8.304	1053	1056	1059	rVB	39627	48056	2.40%	0.383%
9	9.216	1205	1211	1221	rBV	1217300	1591867	79.42%	12.675%
10	9.898	1323	1327	1349	rVB2	617785	1356728	67.69%	10.803%
11	10.616	1444	1449	1457	rVB	84265	110023	5.49%	0.876%
12	10.692	1457	1462	1471	rBV	616712	797263	39.78%	6.348%
13	11.392	1576	1581	1588	rBV	347062	457209	22.81%	3.640%
14	11.910	1664	1669	1680	rBV	124385	192658	9.61%	1.534%
15	12.698	1799	1803	1812	rBV	25081	39971	1.99%	0.318%
16	12.974	1845	1850	1859	rBV	888575	1135583	56.65%	9.042%
17	13.457	1927	1932	1938	rVB	107970	151948	7.58%	1.210%
18	13.863	1997	2001	2009	rBV	70542	103432	5.16%	0.824%
19	14.045	2027	2032	2044	rBV	233890	353118	17.62%	2.812%
20	15.539	2282	2286	2295	rVB	134963	217605	10.86%	1.733%

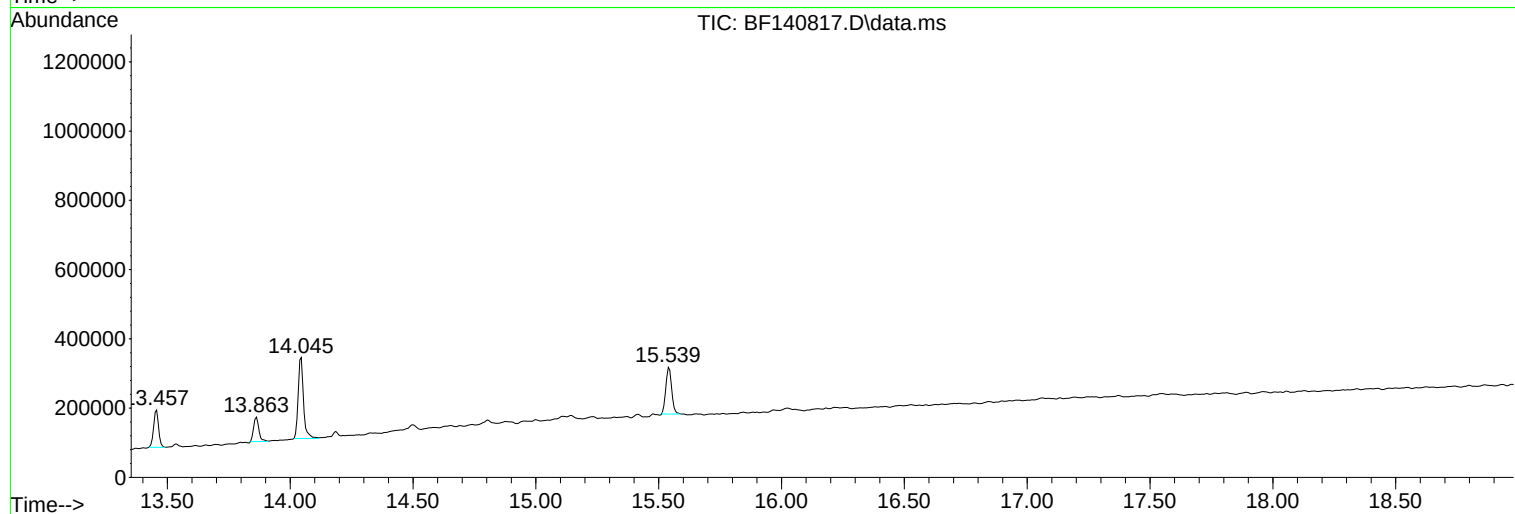
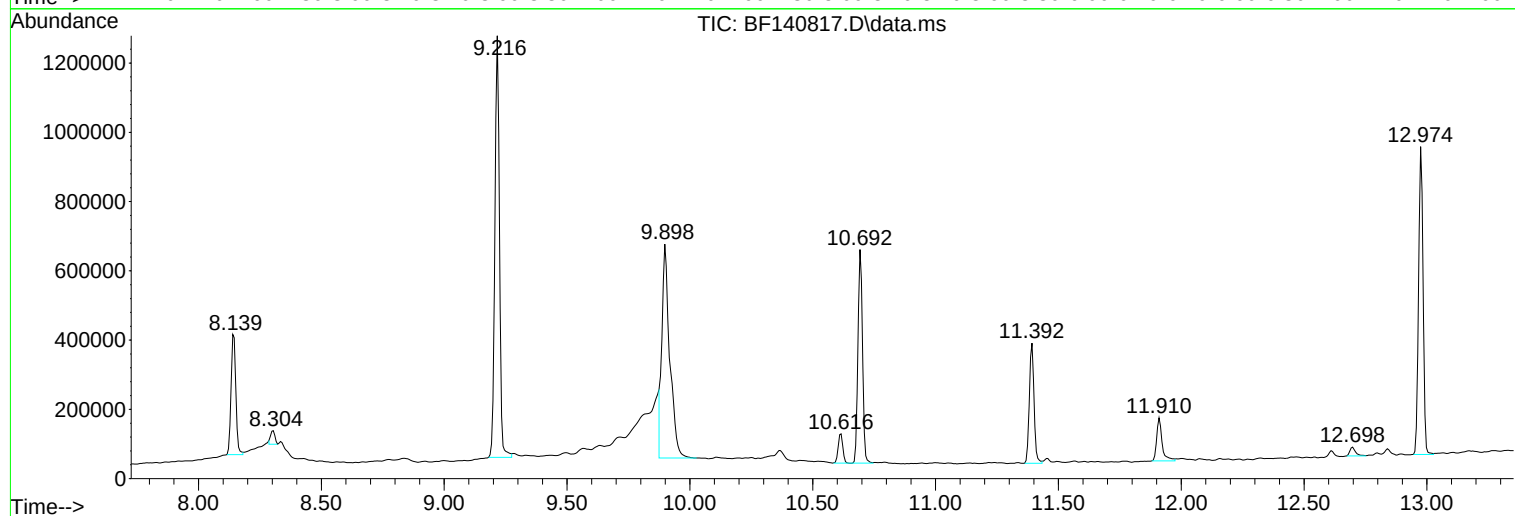
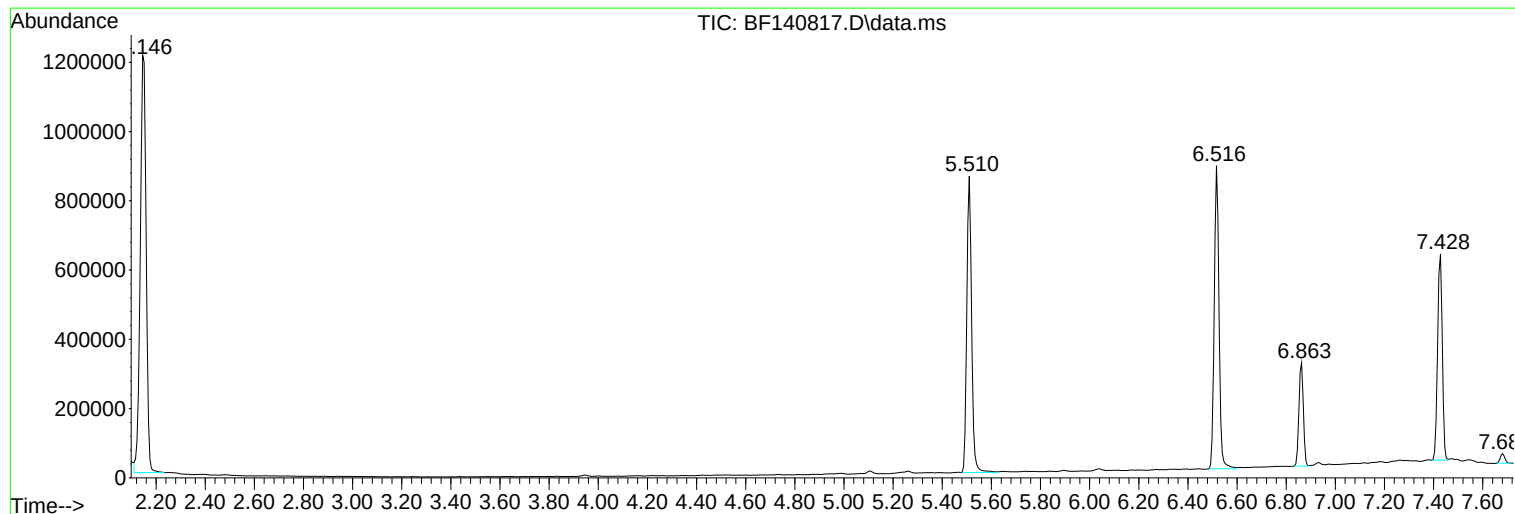
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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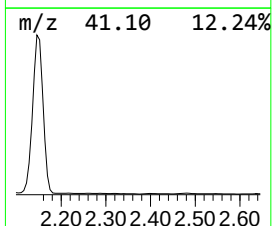
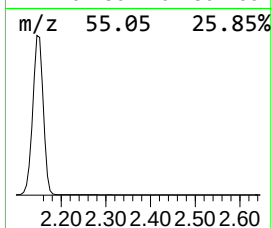
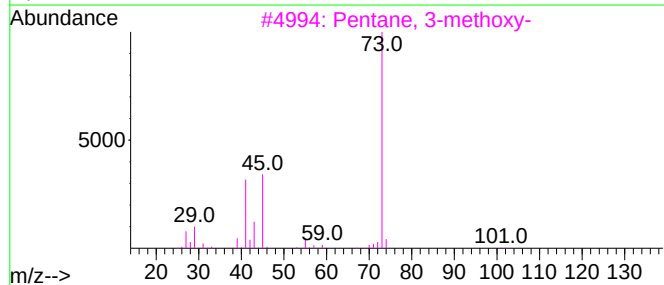
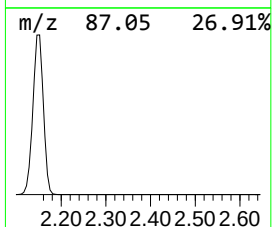
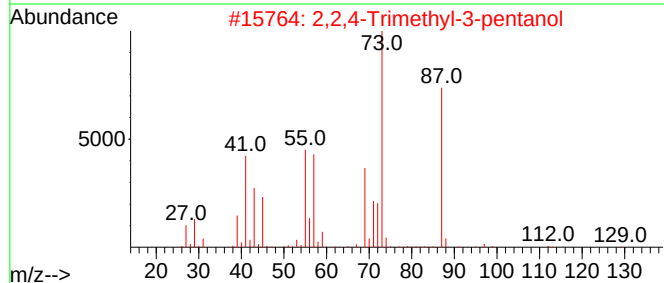
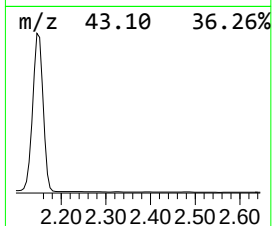
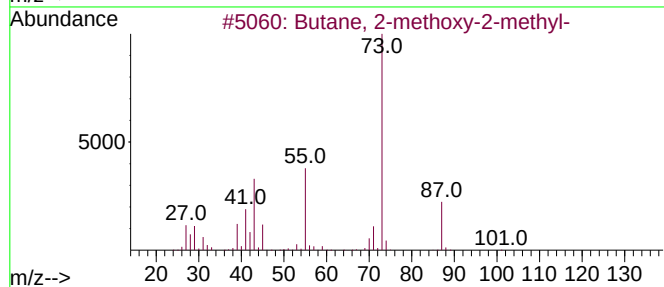
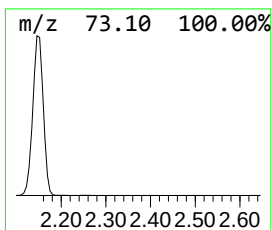
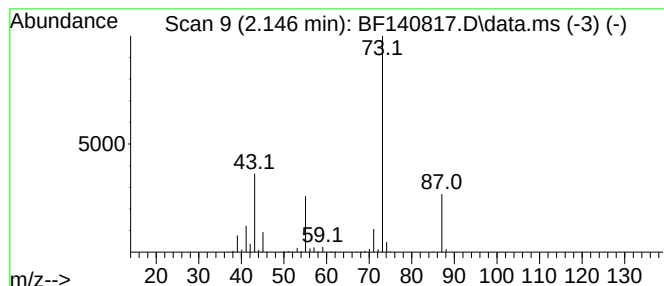
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.146	107.28 ng	2004410	1,4-Dichlorobenzene-d4	6.863

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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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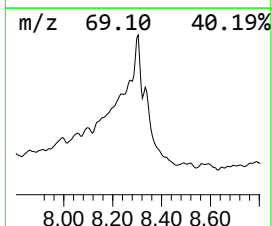
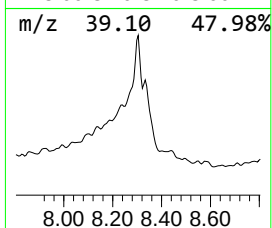
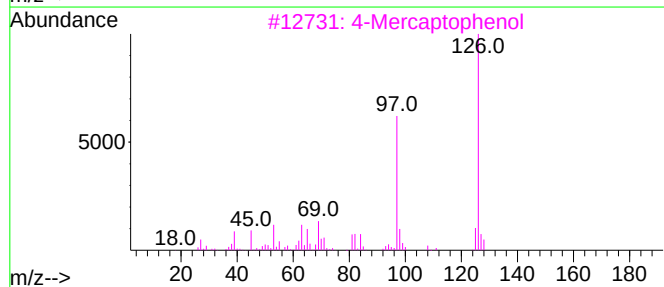
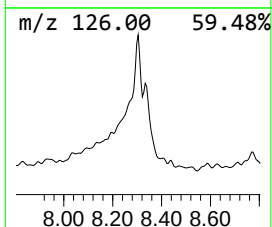
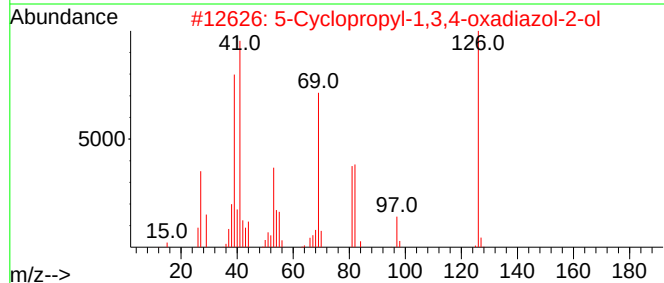
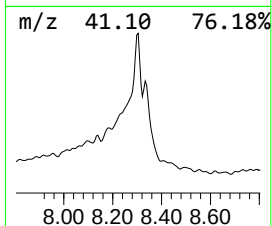
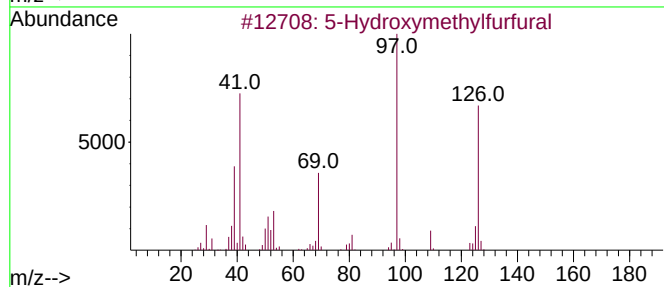
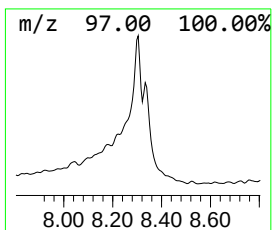
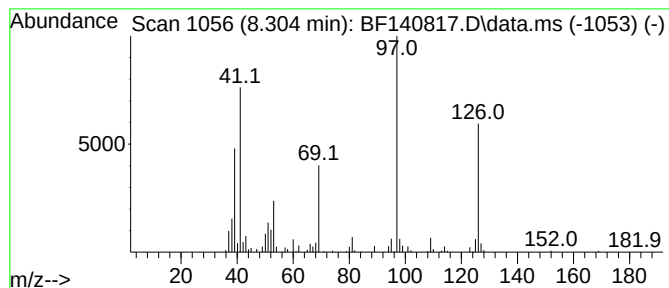
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 5-Hydroxymethylfurfural Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.304	2.05 ng	48056	Naphthalene-d8	8.139

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Hydroxymethylfurfural	126	C6H6O3	000067-47-0	90
2		5-Cyclopropyl-1,3,4-oxadiazol-2-ol	126	C5H6N2O2	1000445-07-9	53
3		4-Mercaptophenol	126	C6H6OS	000637-89-8	43
4		1,2,4-Benzenetriol	126	C6H6O3	000533-73-3	27
5		2-Fluoropyridine	97	C5H4FN	000372-48-5	25



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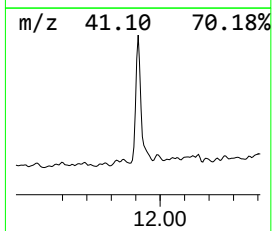
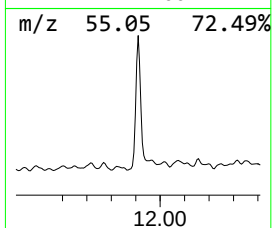
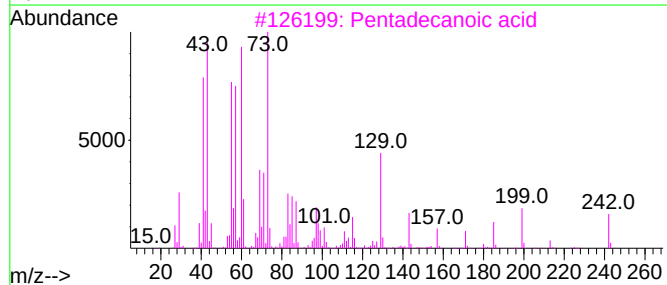
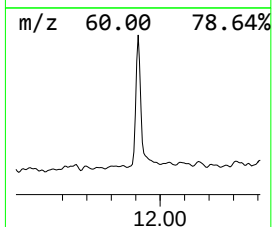
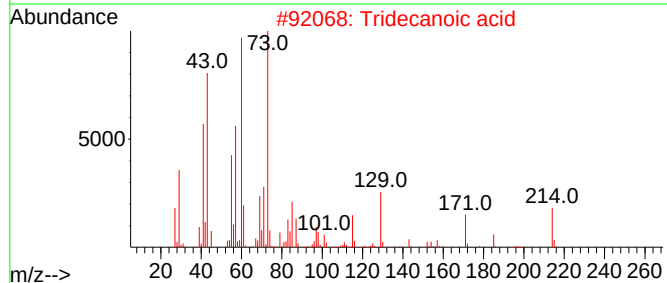
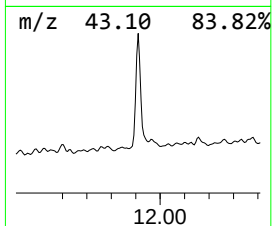
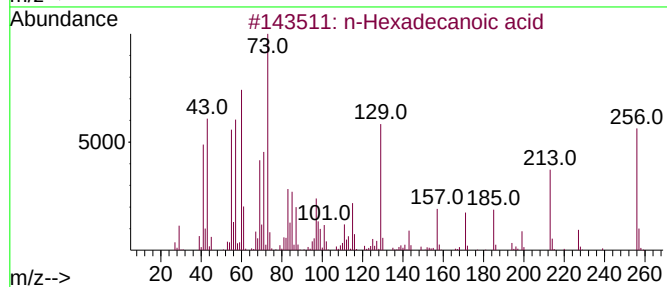
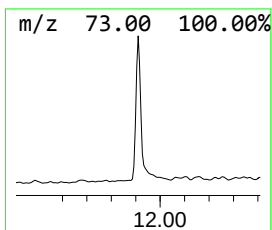
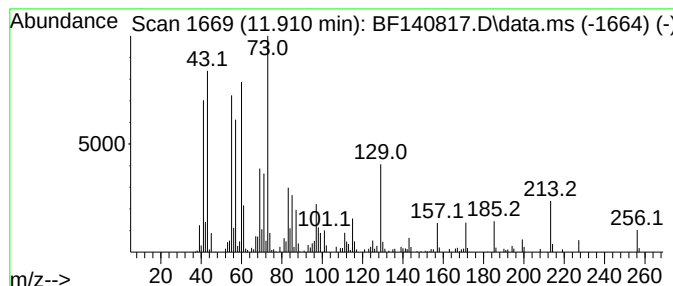
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.910	8.43 ng	192658	Phenanthrene-d10	11.392	
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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68



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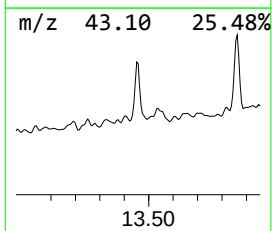
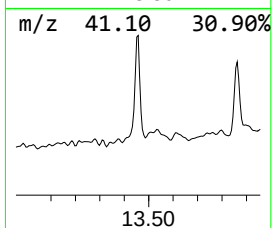
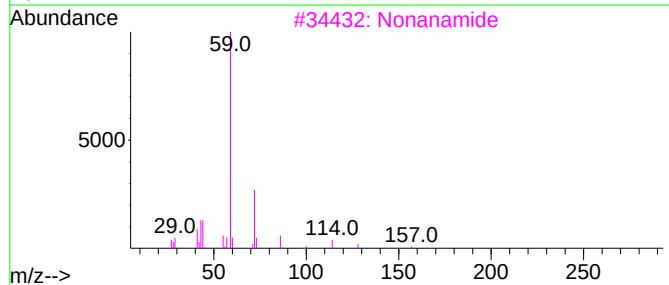
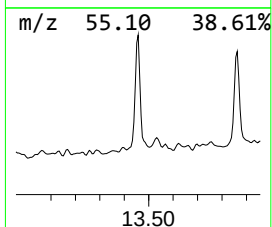
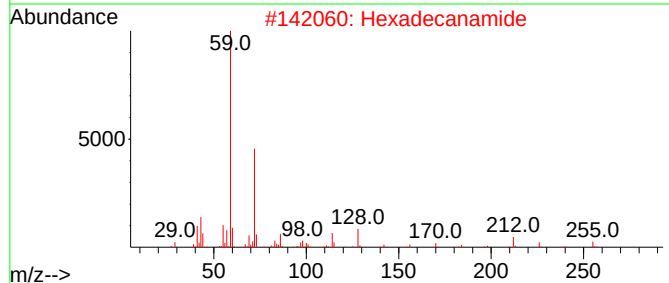
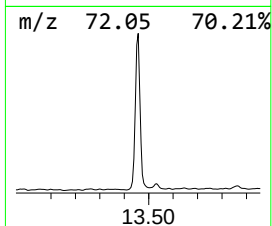
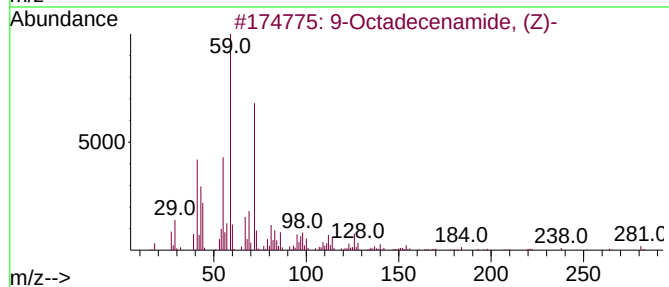
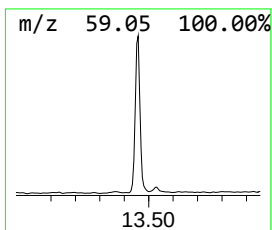
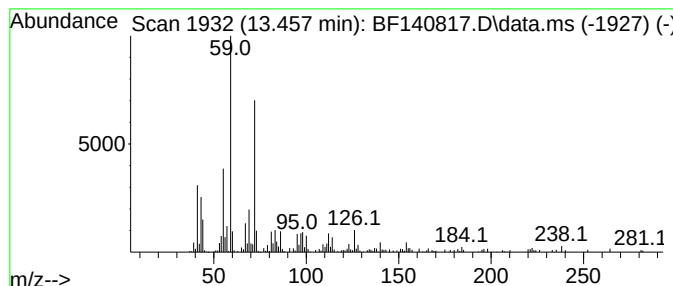
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	8.61 ng	151948	Chrysene-d12	14.045

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		Hexadecanamide	255	C16H33NO	000629-54-9	72
3		Nonanamide	157	C9H19NO	001120-07-6	64
4		Octanamide	143	C8H17NO	000629-01-6	59
5		7-Nonenamide	155	C9H17NO	090949-53-4	58



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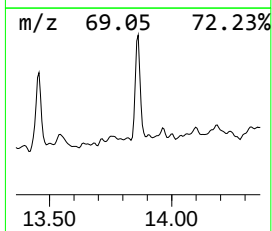
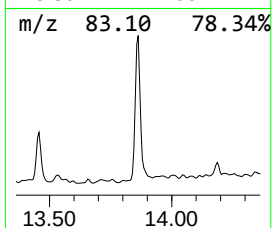
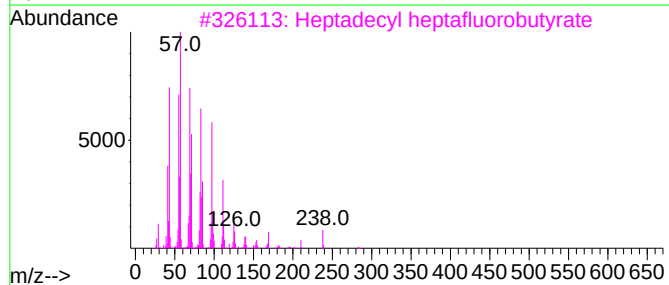
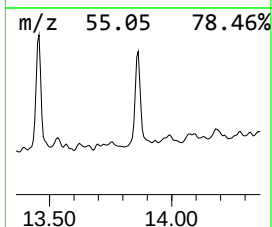
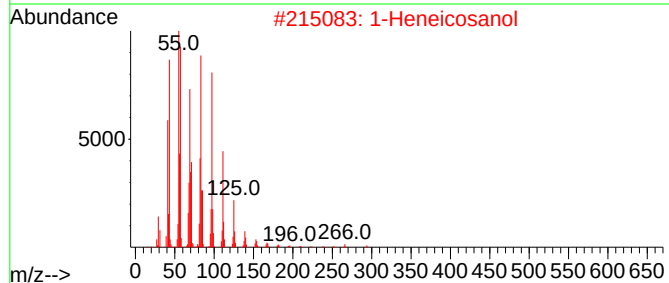
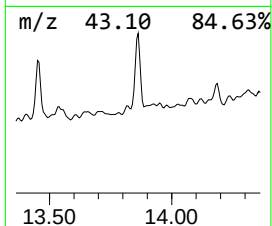
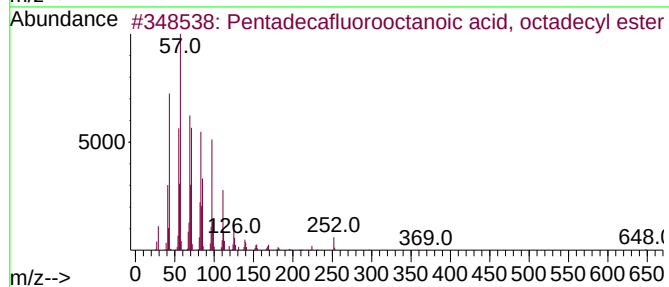
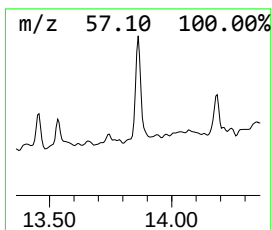
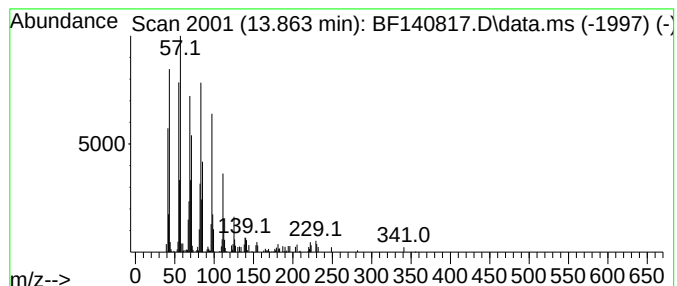
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.863	5.86 ng	103432	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	107.3	ng	2004410	1	6.863	373685	20.0
5-Hydroxymethyl...	8.304	2.0	ng	48056	2	8.139	469883	20.0
n-Hexadecanoic ...	11.910	8.4	ng	192658	4	11.392	457209	20.0
9-Octadecenamid...	13.457	8.6	ng	151948	5	14.045	353118	20.0
Pentadecafluoro...	13.863	5.9	ng	103432	5	14.045	353118	20.0