

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063023\
 Data File : BF134069.D
 Acq On : 01 Jul 2023 00:56
 Operator : CG\JU
 Sample : 03428-03 2X
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PNNL-APM-0621-2

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: BF134069.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	19	23	34	rVB	21832	37577	2.63%	0.354%
2	5.075	504	508	518	rBV	54830	61932	4.34%	0.584%
3	5.475	572	576	592	rBV	1284444	1179039	82.56%	11.119%
4	6.475	742	746	759	rBV	1232260	1178545	82.52%	11.115%
5	6.845	805	809	816	rBV	763732	615680	43.11%	5.806%
6	7.404	900	904	916	rBV	957047	778969	54.54%	7.346%
7	8.122	1023	1026	1030	rBV	921361	753991	52.79%	7.111%
8	9.198	1206	1209	1213	rBV	1726732	1428183	100.00%	13.469%
9	9.880	1322	1325	1329	rBV	934405	757963	53.07%	7.148%
10	10.598	1443	1447	1456	rBV	250955	207210	14.51%	1.954%
11	10.675	1456	1460	1471	rBV	719849	671811	47.04%	6.336%
12	10.910	1497	1500	1504	rBV	44154	39822	2.79%	0.376%
13	11.374	1575	1579	1587	rBV	737811	643440	45.05%	6.068%
14	11.904	1666	1669	1674	rBV2	62598	67028	4.69%	0.632%
15	12.968	1847	1850	1854	rBV	1062279	1007923	70.57%	9.506%
16	13.904	2005	2009	2019	rVB7	42071	92270	6.46%	0.870%
17	14.033	2027	2031	2037	rBV	560086	561542	39.32%	5.296%
18	15.539	2283	2287	2291	rBV	351125	467649	32.74%	4.410%
19	16.033	2369	2371	2376	rVB2	40412	53000	3.71%	0.500%

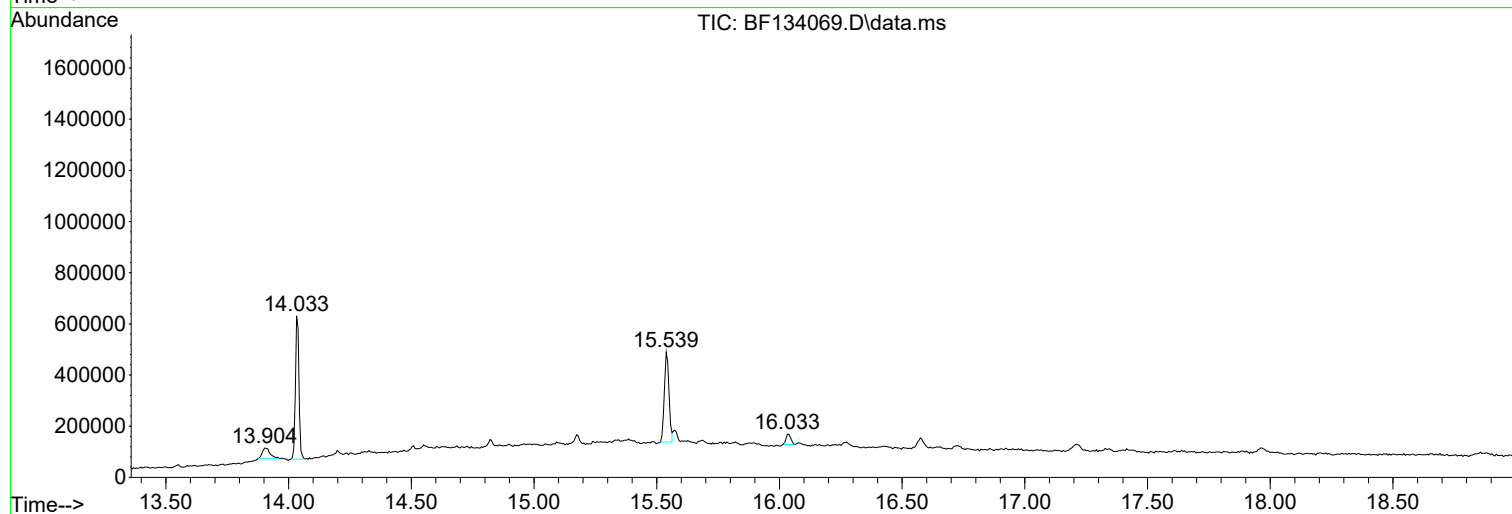
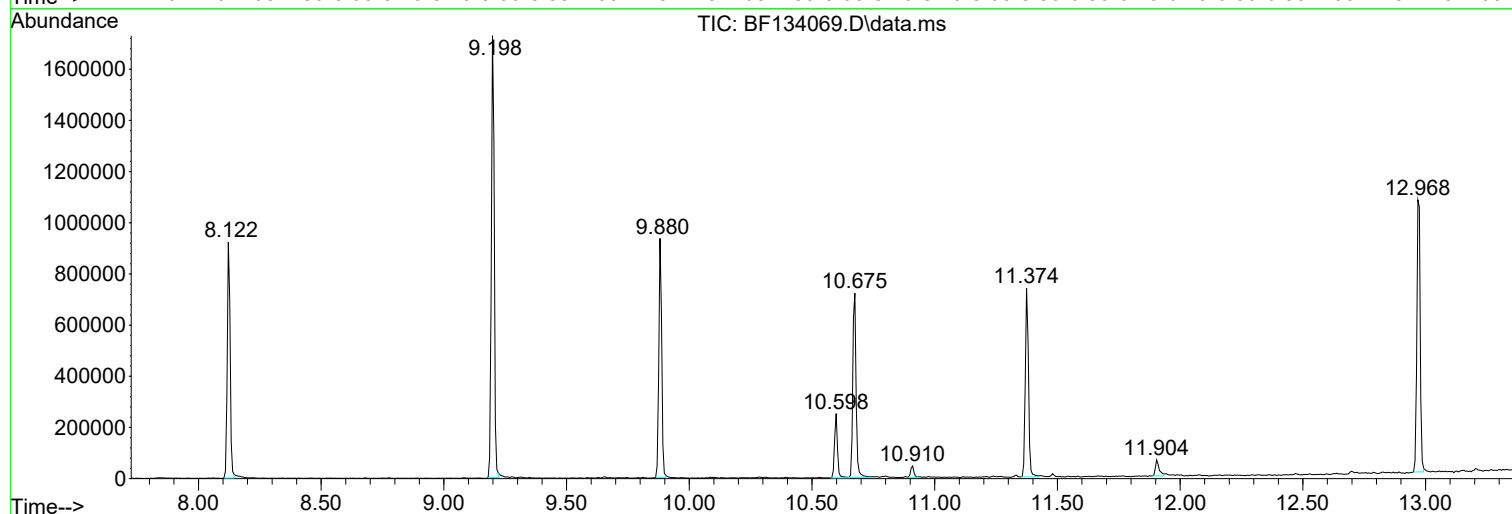
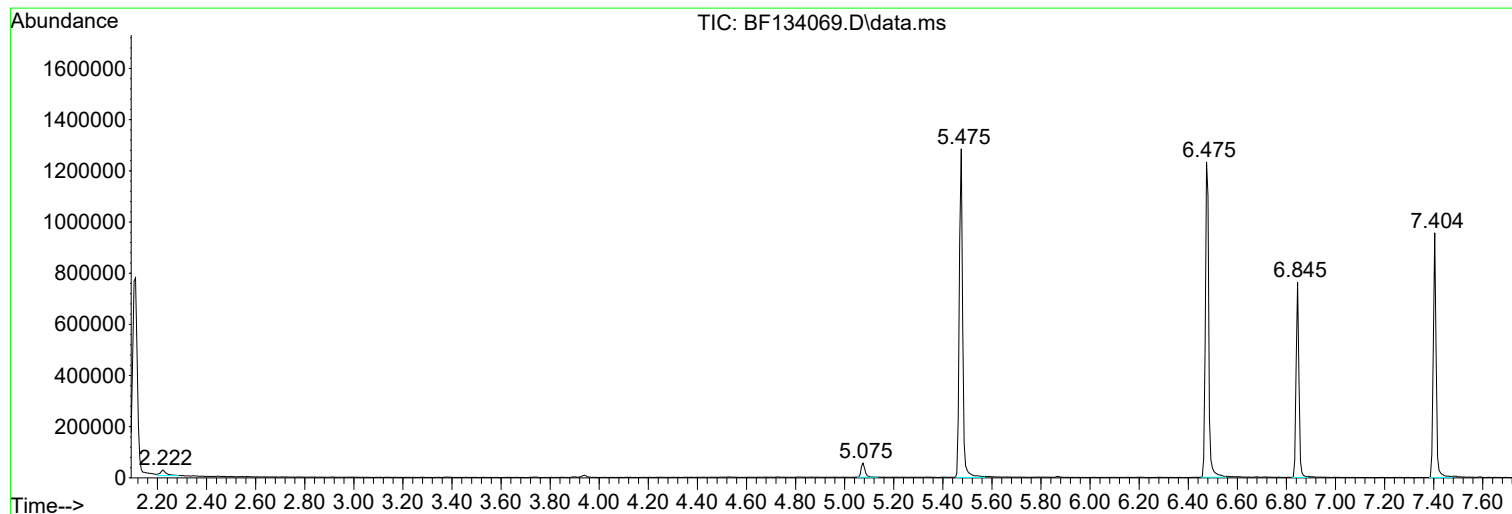
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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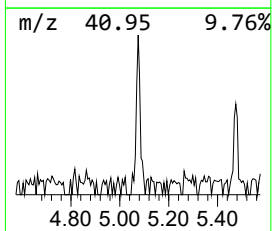
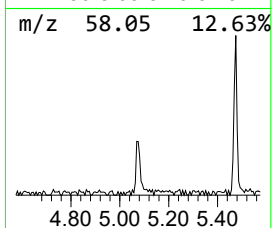
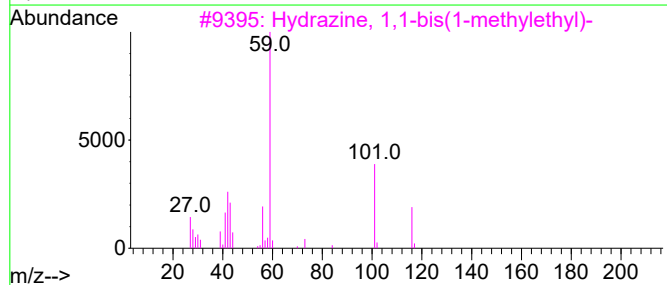
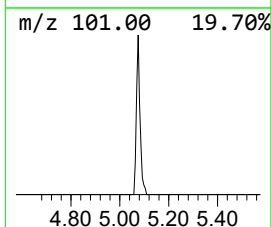
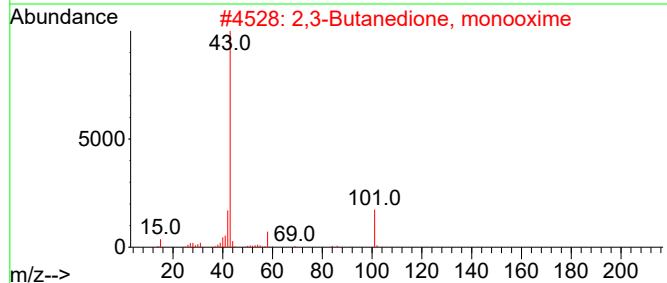
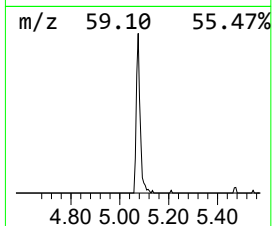
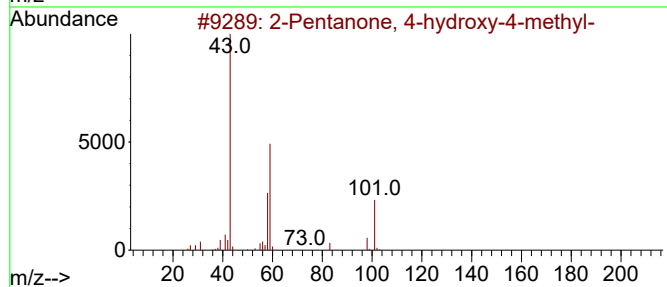
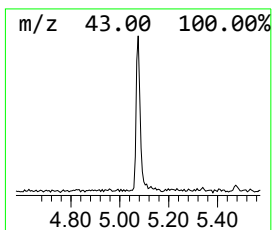
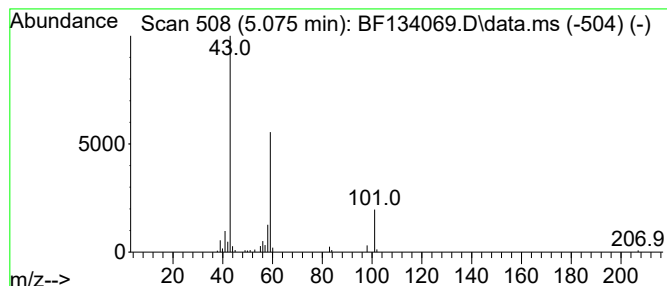
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	2.01 ng	61932	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	72		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38		
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	23		



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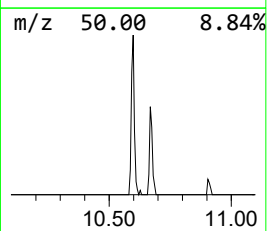
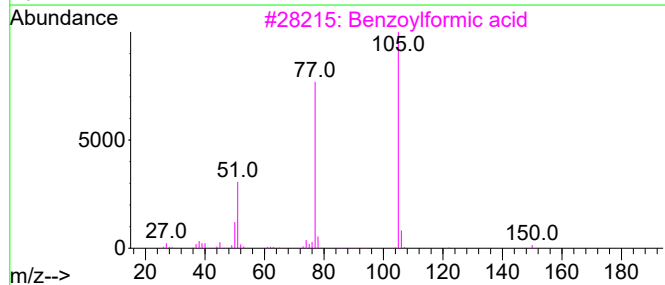
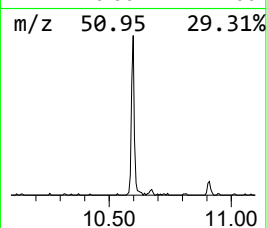
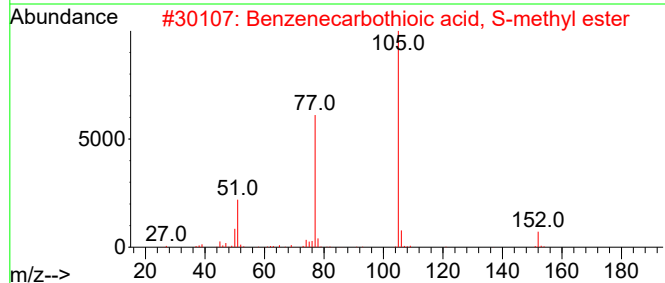
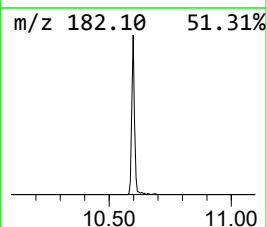
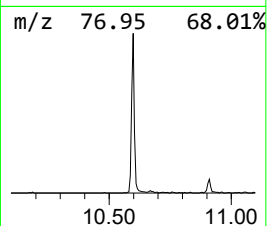
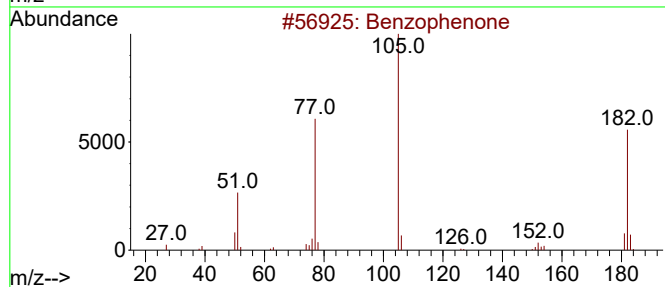
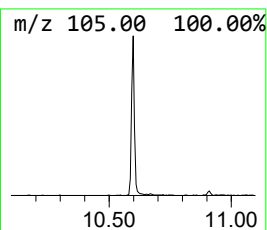
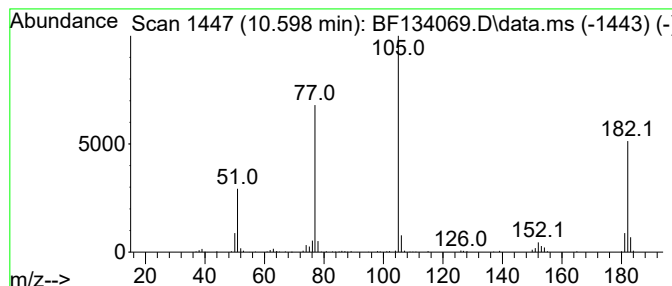
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	5.47 ng	207210	Acenaphthene-d10	9.880

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			Benzoylformic acid	150	C8H6O3	000611-73-4	53
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
5			Benzoic acid, ethyl ester	150	C9H10O2	000093-89-0	47



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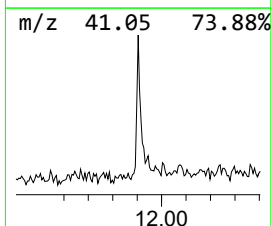
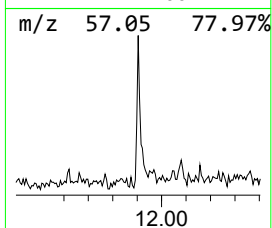
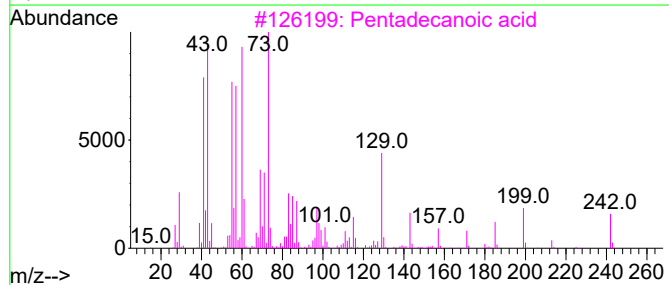
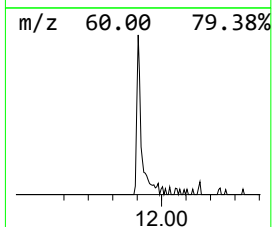
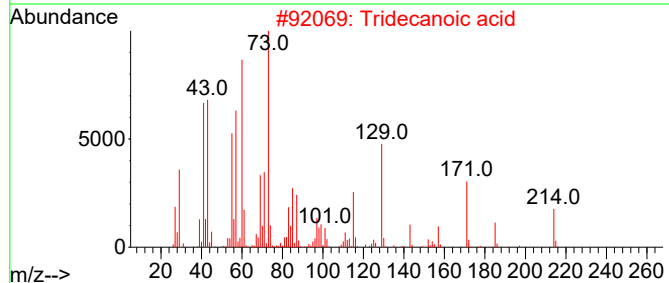
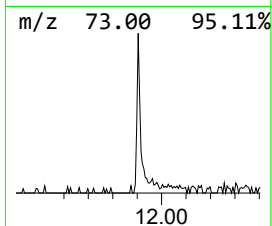
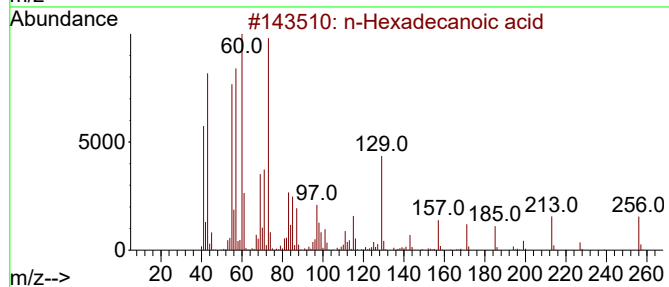
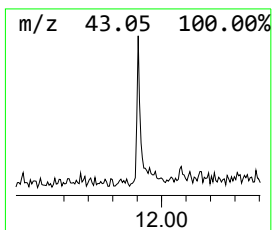
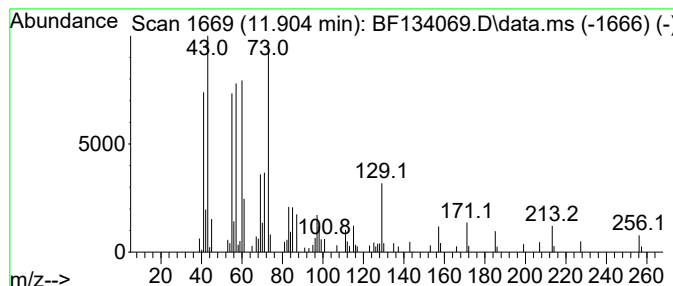
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	2.08 ng	67028	Phenanthrene-d10	11.374

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	70
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Isopropyl palmitate	298	C19H38O2	000142-91-6	58
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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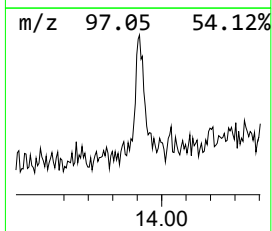
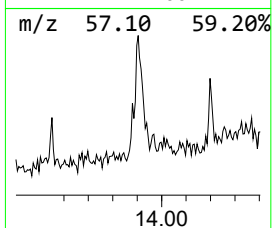
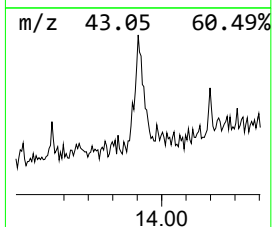
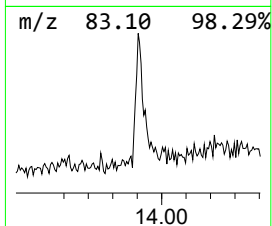
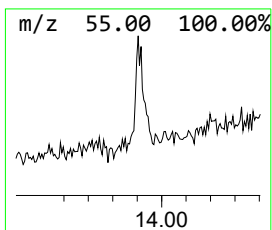
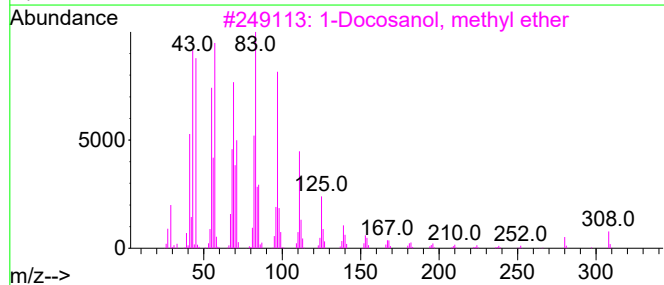
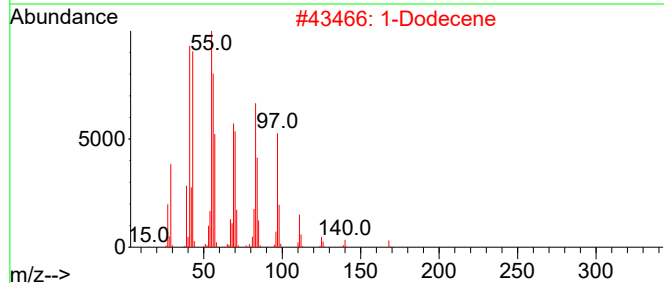
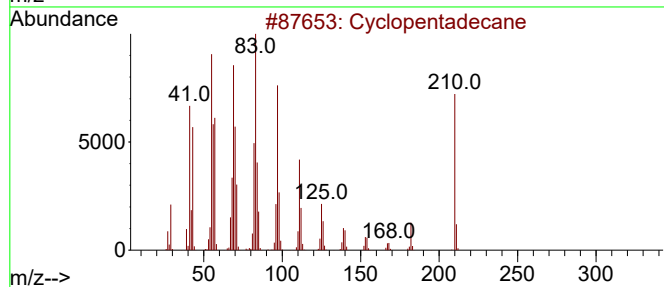
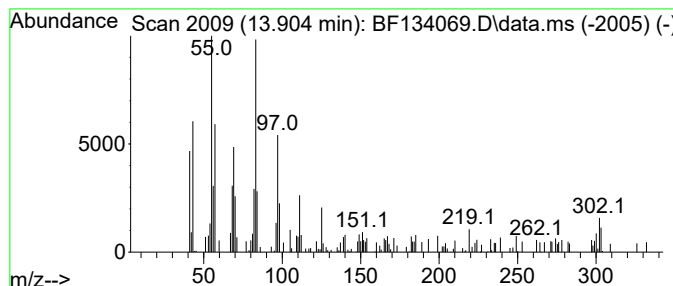
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.29 ng	92270	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	78
2			1-Dodecene	168	C12H24	000112-41-4	52
3			1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	49
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	49
5			1,3-Cyclohexanedione, 5,5-dimeth...	182	C11H18O2	001919-64-8	49



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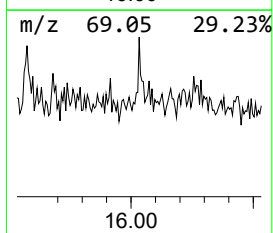
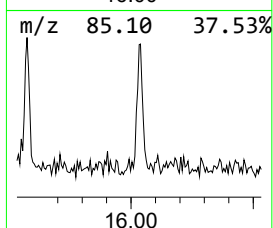
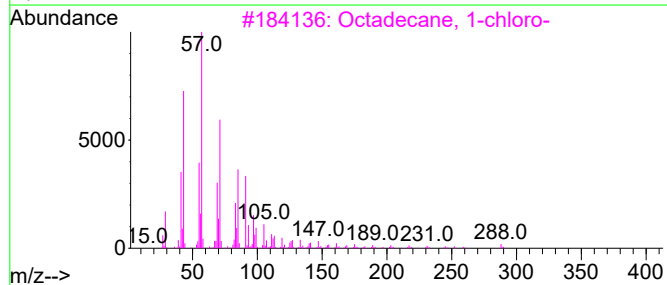
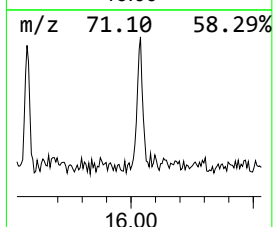
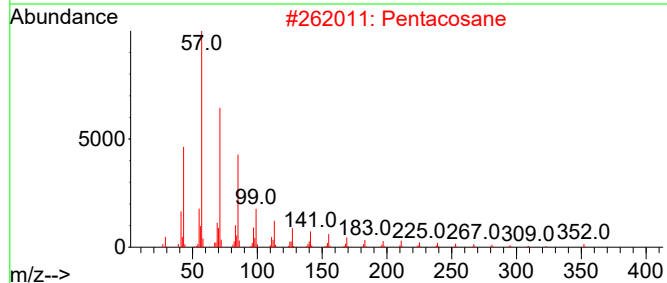
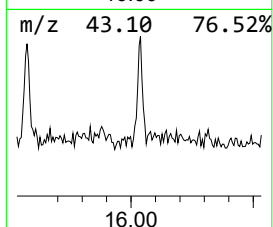
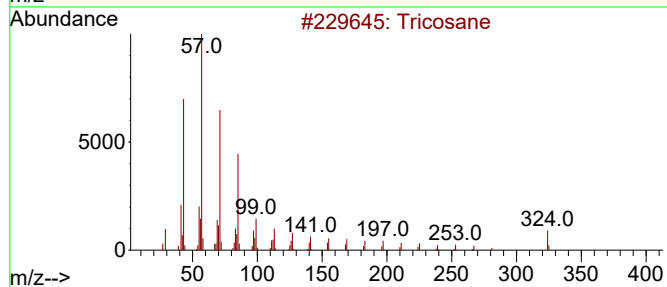
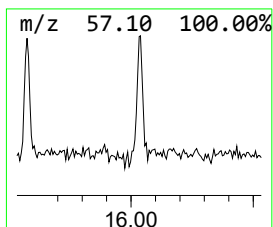
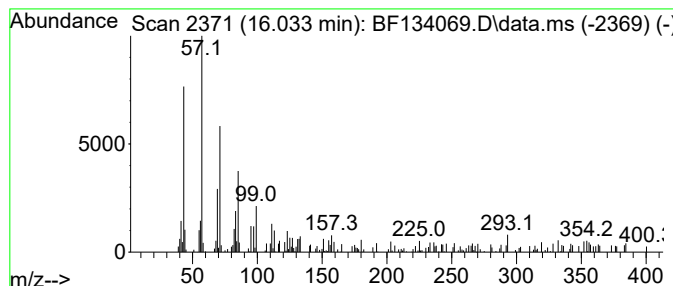
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tricosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	2.27 ng	53000	Perylene-d12	15.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	60
2			Pentacosane	352	C25H52	000629-99-2	60
3			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	60
4			Docosane	310	C22H46	000629-97-0	60
5			Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.075	2.0	ng	61932	1	6.845	615680	20.0
Benzophenone	10.598	5.5	ng	207210	3	9.880	757963	20.0
n-Hexadecanoic ...	11.904	2.1	ng	67028	4	11.374	643440	20.0
Cyclopentadecane	13.904	3.3	ng	92270	5	14.033	561542	20.0
Tricosane	16.033	2.3	ng	53000	6	15.539	467649	20.0