

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
 Data File : BF134109.D
 Acq On : 06 Jul 2023 21:53
 Operator : CG\JU
 Sample : 03475-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ALDENE-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: BF134109.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	8	13	28	rVB	1062411	1418437	60.70%	8.055%
2	2.275	29	32	41	rVB	33492	54580	2.34%	0.310%
3	5.093	507	511	521	rVB	109478	144821	6.20%	0.822%
4	5.481	573	577	590	rBV	2032382	1974182	84.48%	11.211%
5	6.481	742	747	750	rBV	2138849	1929647	82.58%	10.958%
6	6.845	805	809	819	rBV	682954	557758	23.87%	3.167%
7	7.410	900	905	916	rBV	1282781	1303654	55.79%	7.403%
8	8.122	1023	1026	1040	rBV	844426	730641	31.27%	4.149%
9	9.204	1206	1210	1213	rBV	2609523	2302413	98.53%	13.075%
10	9.880	1322	1325	1331	rBV	990193	785675	33.62%	4.462%
11	10.598	1444	1447	1456	rBV	206180	164743	7.05%	0.936%
12	10.674	1456	1460	1472	rBV	1798252	1609508	68.88%	9.140%
13	10.910	1497	1500	1504	rVB	28844	26218	1.12%	0.149%
14	11.374	1575	1579	1587	rBV	953688	837411	35.84%	4.756%
15	11.904	1666	1669	1674	rBV	111550	116650	4.99%	0.662%
16	12.974	1847	1851	1854	rBV	2727470	2336730	100.00%	13.270%
17	13.921	2007	2012	2026	rBV6	41234	130380	5.58%	0.740%
18	14.033	2027	2031	2039	rVB	672053	648100	27.74%	3.680%
19	14.898	2174	2178	2181	rVB2	25279	31625	1.35%	0.180%
20	15.539	2282	2287	2296	rVB	373449	506096	21.66%	2.874%

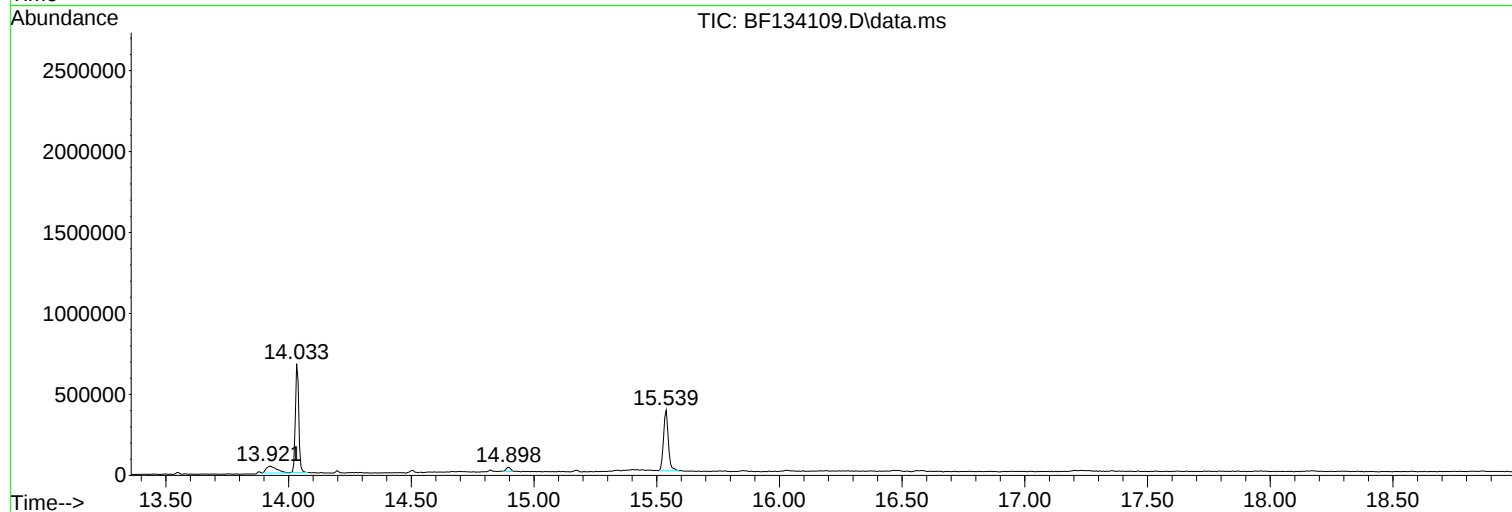
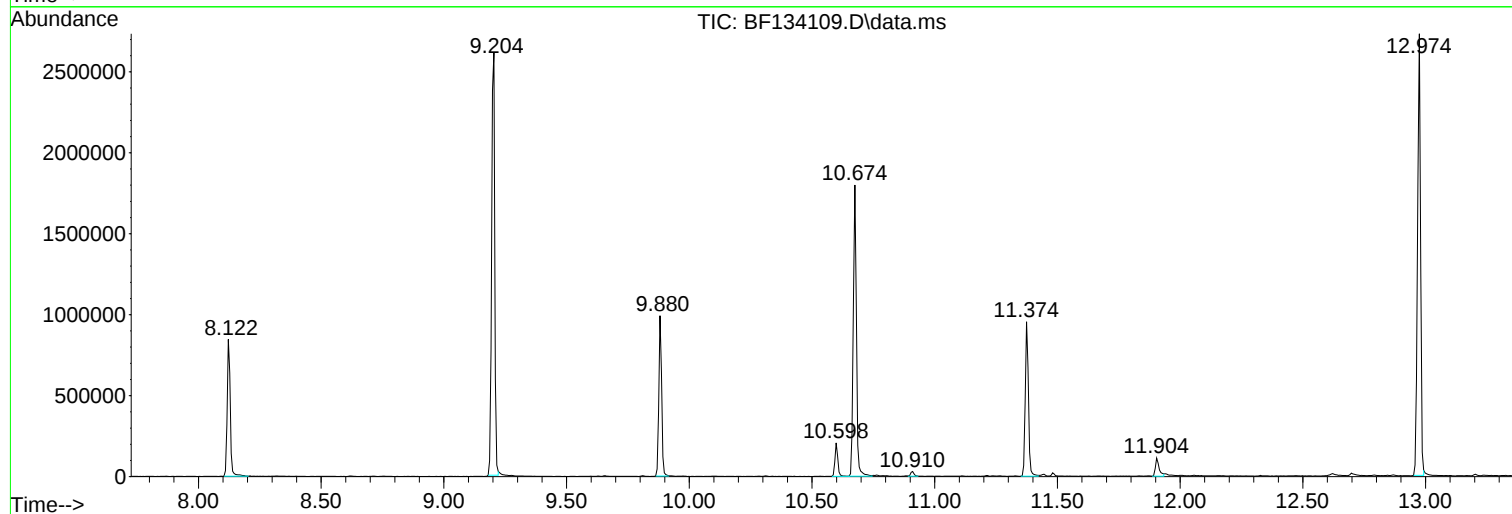
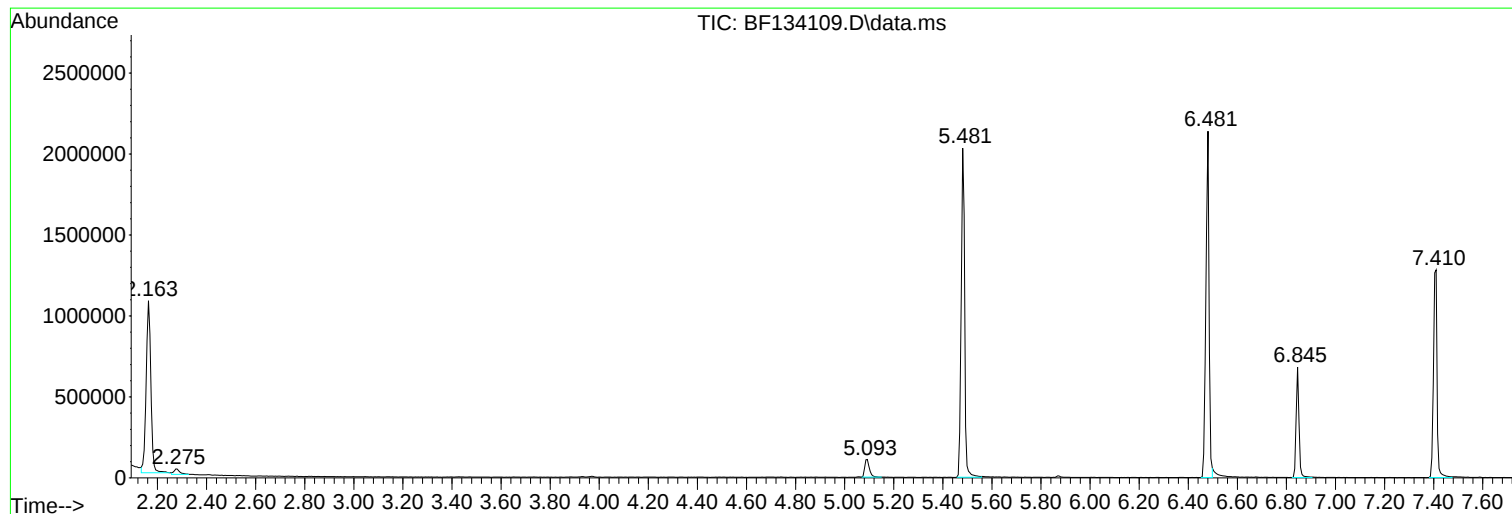
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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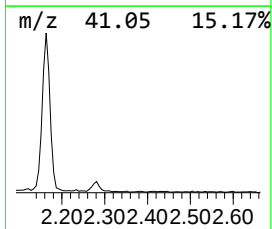
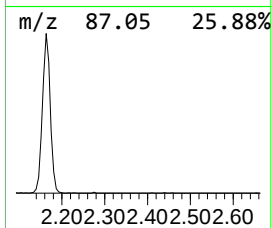
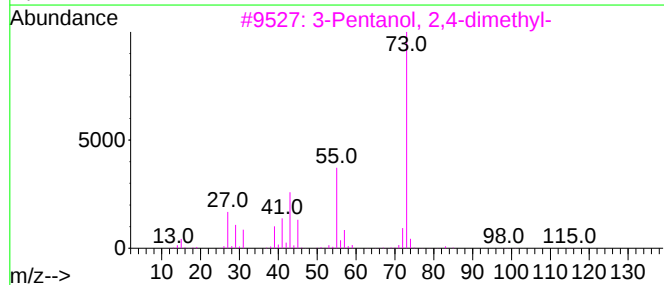
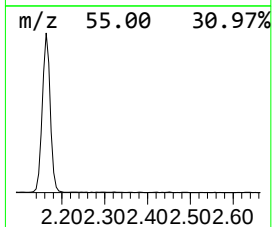
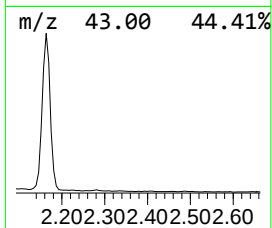
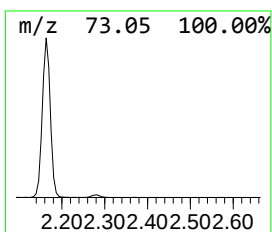
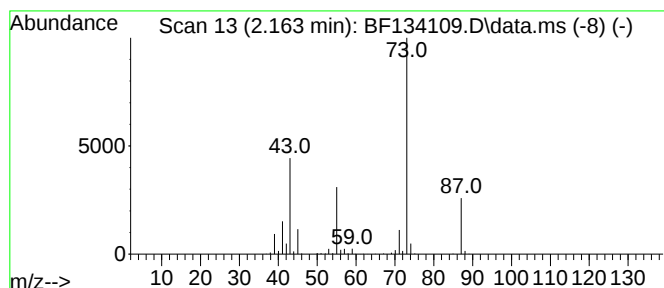
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	50.86 ng	1418440	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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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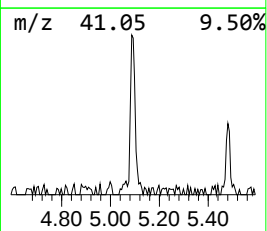
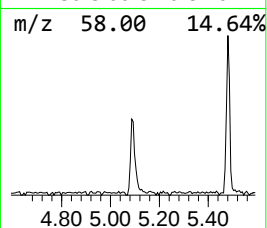
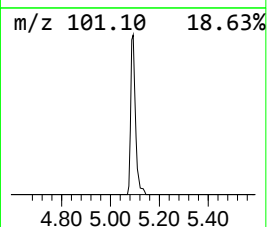
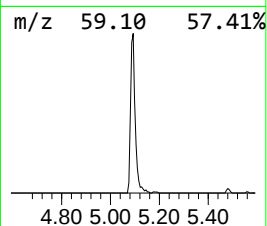
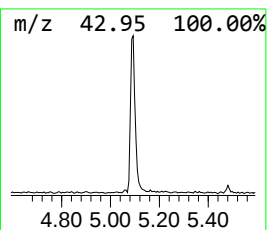
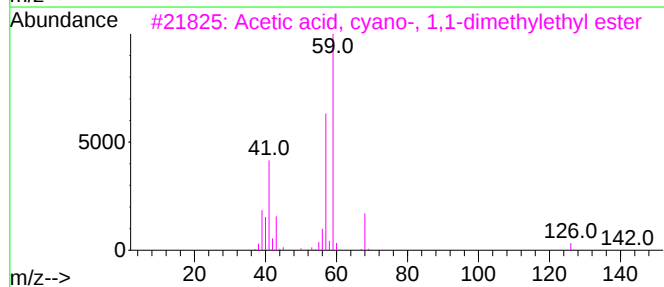
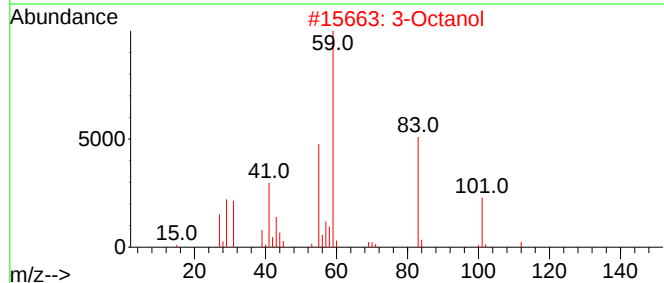
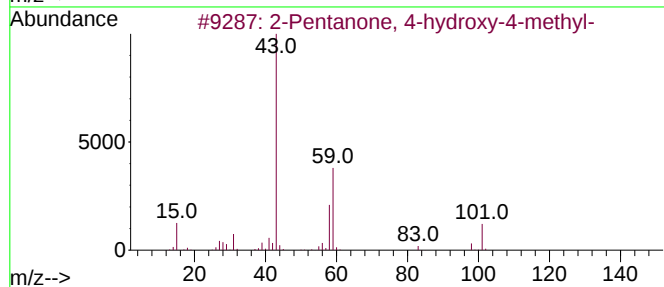
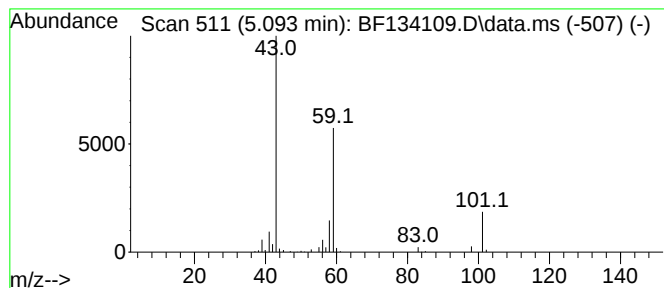
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	5.19 ng	144821	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	50		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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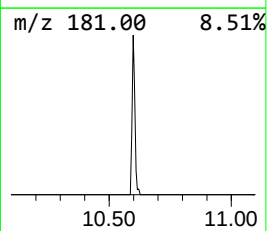
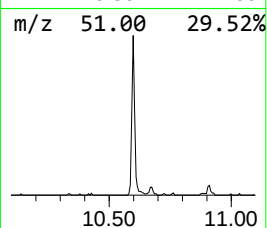
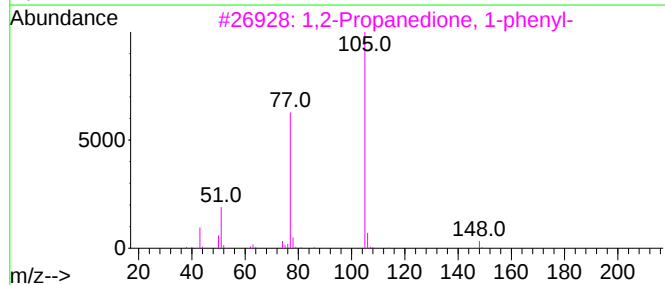
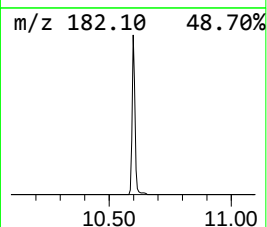
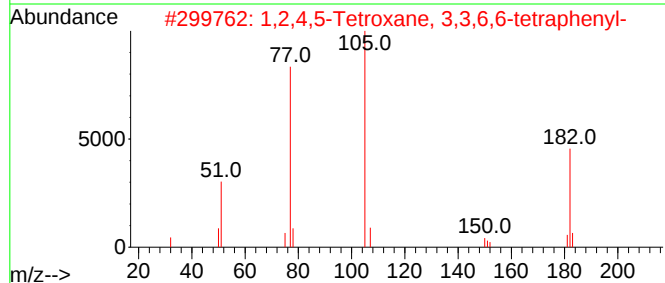
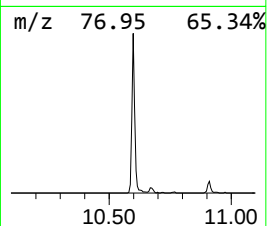
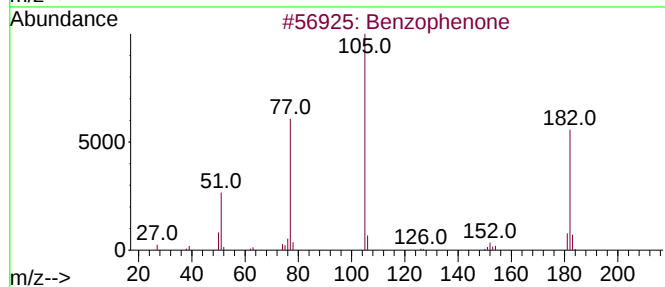
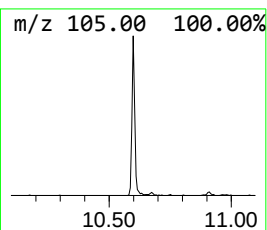
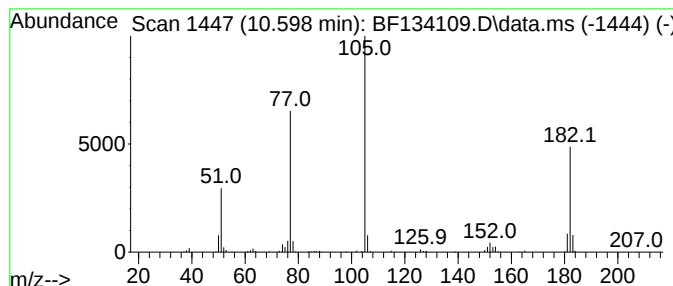
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	4.19 ng	164743	Acenaphthene-d10	9.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	59
3			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47



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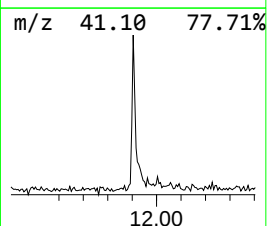
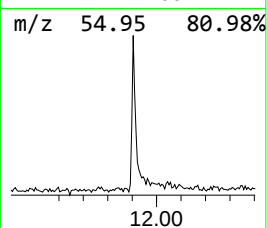
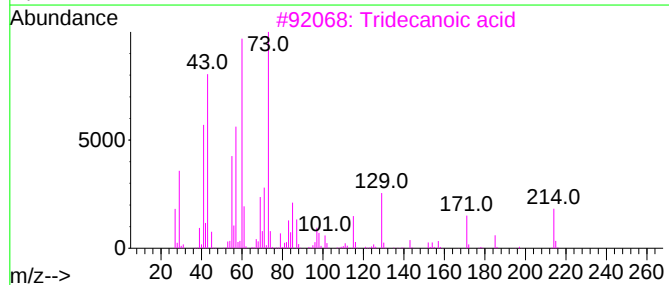
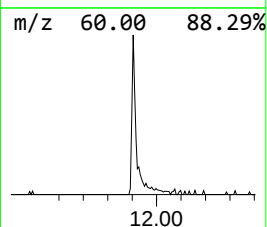
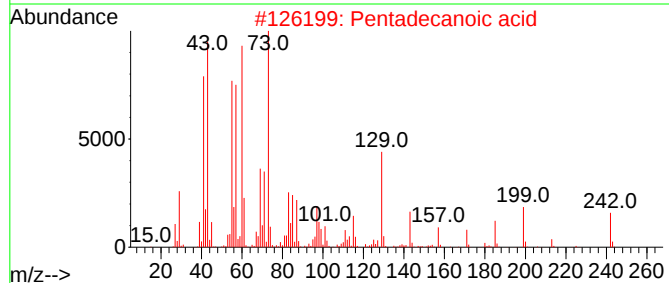
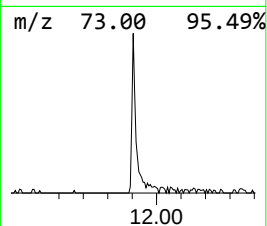
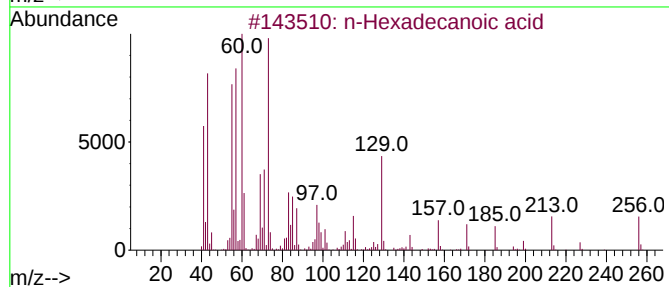
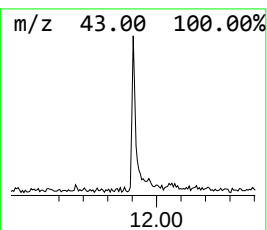
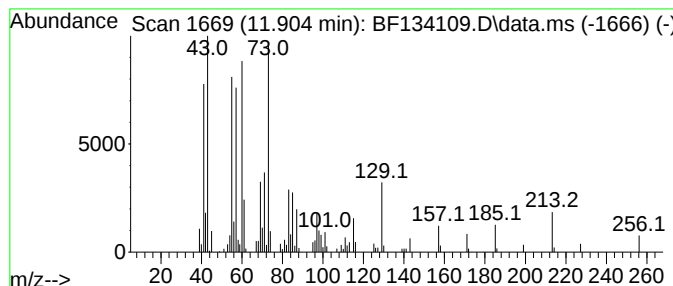
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	2.79 ng	116650	Phenanthrene-d10	11.374

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Dodecanoic acid	200	C12H24O2	000143-07-7	72
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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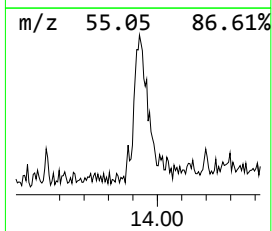
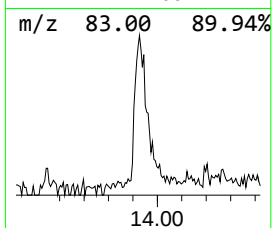
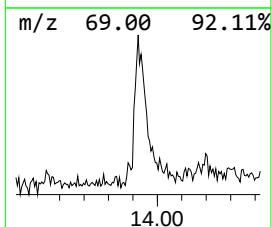
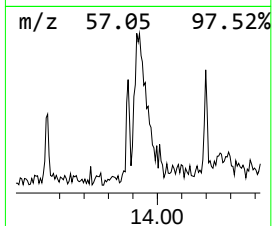
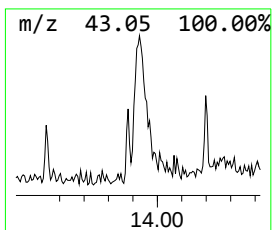
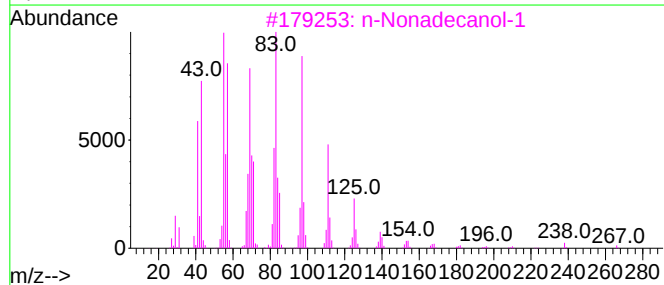
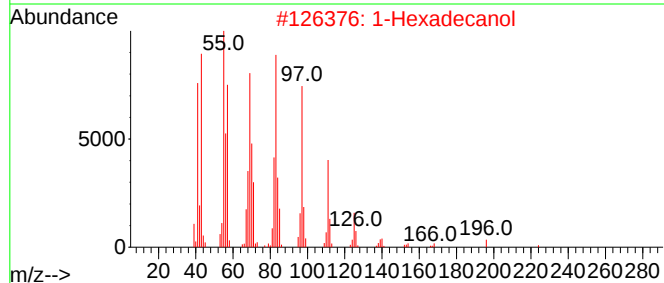
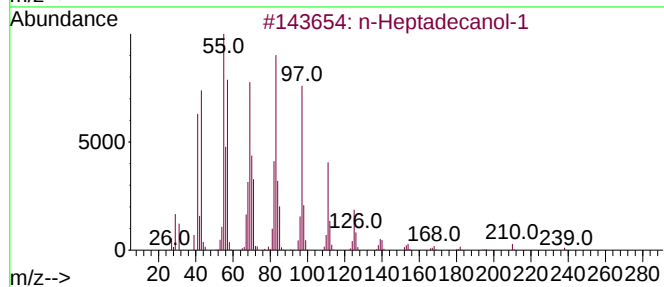
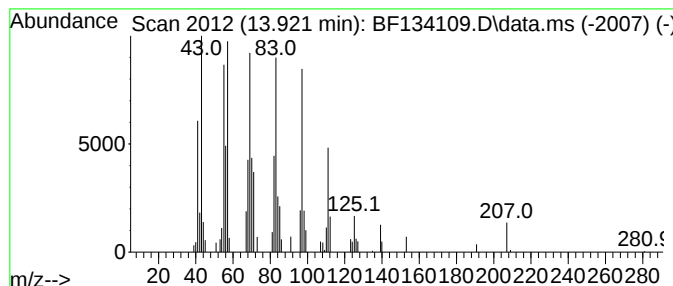
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Peak Number 5 n-Heptadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.921	4.02 ng	130380	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Heptadecanol-1	256	C17H36O	001454-85-9	91
2			1-Hexadecanol	242	C16H34O	036653-82-4	91
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			1-Octadecanol	270	C18H38O	000112-92-5	90
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.163	50.9	ng	1418440	1	6.845	557758	20.0
2-Pentanone, 4-...	5.093	5.2	ng	144821	1	6.845	557758	20.0
Benzophenone	10.598	4.2	ng	164743	3	9.880	785675	20.0
n-Hexadecanoic ...	11.904	2.8	ng	116650	4	11.374	837411	20.0
n-Heptadecanol-1	13.921	4.0	ng	130380	5	14.033	648100	20.0