

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
 Data File : BF134398.D
 Acq On : 21 Jul 2023 13:24
 Operator : CG\JU
 Sample : 03638-21
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP6

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: BF134398.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	13	rVB	314747	326674	25.75%	3.141%
2	5.081	505	509	517	rBV	15114	21464	1.69%	0.206%
3	5.469	572	575	587	rBV	987588	1011803	79.77%	9.729%
4	6.475	742	746	766	rBV	1177286	1044079	82.31%	10.039%
5	6.833	804	807	819	rBV	424750	365830	28.84%	3.518%
6	7.398	899	903	916	rBV	783726	682894	53.84%	6.566%
7	8.116	1021	1025	1042	rBV	549137	480651	37.89%	4.622%
8	9.192	1204	1208	1211	rBV	1646484	1268442	100.00%	12.196%
9	9.874	1320	1324	1327	rBV	630846	530592	41.83%	5.102%
10	10.010	1344	1347	1357	rBV	162815	162802	12.83%	1.565%
11	10.669	1455	1459	1475	rBV	956395	875727	69.04%	8.420%
12	11.368	1574	1578	1581	rBV	697600	569067	44.86%	5.472%
13	11.392	1581	1582	1587	rVB	50705	29794	2.35%	0.286%
14	11.898	1665	1668	1676	rBV3	204485	184209	14.52%	1.771%
15	12.592	1783	1786	1789	rBV	101434	88460	6.97%	0.851%
16	12.686	1800	1802	1810	rBV2	33378	43224	3.41%	0.416%
17	12.821	1820	1825	1829	rBV	91036	86201	6.80%	0.829%
18	12.968	1845	1850	1853	rBV	1326856	1266119	99.82%	12.174%
19	13.539	1943	1947	1949	rBV2	23921	21832	1.72%	0.210%
20	13.868	2000	2003	2007	rBV2	30112	31259	2.46%	0.301%
21	13.933	2007	2014	2023	rVV7	34504	108809	8.58%	1.046%
22	14.033	2026	2031	2034	rVV	510435	503543	39.70%	4.842%
23	14.057	2034	2035	2039	rVB	45924	30846	2.43%	0.297%
24	14.186	2054	2057	2063	rVB2	30460	30203	2.38%	0.290%
25	14.498	2105	2110	2112	rBV	29739	32028	2.52%	0.308%
26	14.809	2160	2163	2166	rBV	19328	19462	1.53%	0.187%
27	14.962	2185	2189	2194	rVB4	20101	20815	1.64%	0.200%
28	15.098	2207	2212	2214	rBV	32653	44638	3.52%	0.429%
29	15.156	2219	2222	2227	rVB3	21179	27903	2.20%	0.268%
30	15.409	2261	2265	2271	rVB	18620	25589	2.02%	0.246%
31	15.474	2273	2276	2282	rVV	22672	29104	2.29%	0.280%
32	15.539	2282	2287	2299	rVV	270425	369597	29.14%	3.554%
33	16.009	2363	2367	2372	rVB5	14981	24498	1.93%	0.236%
34	17.086	2545	2550	2557	rVB4	10397	23381	1.84%	0.225%
35	17.556	2626	2630	2637	rVB3	8696	18583	1.47%	0.179%

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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

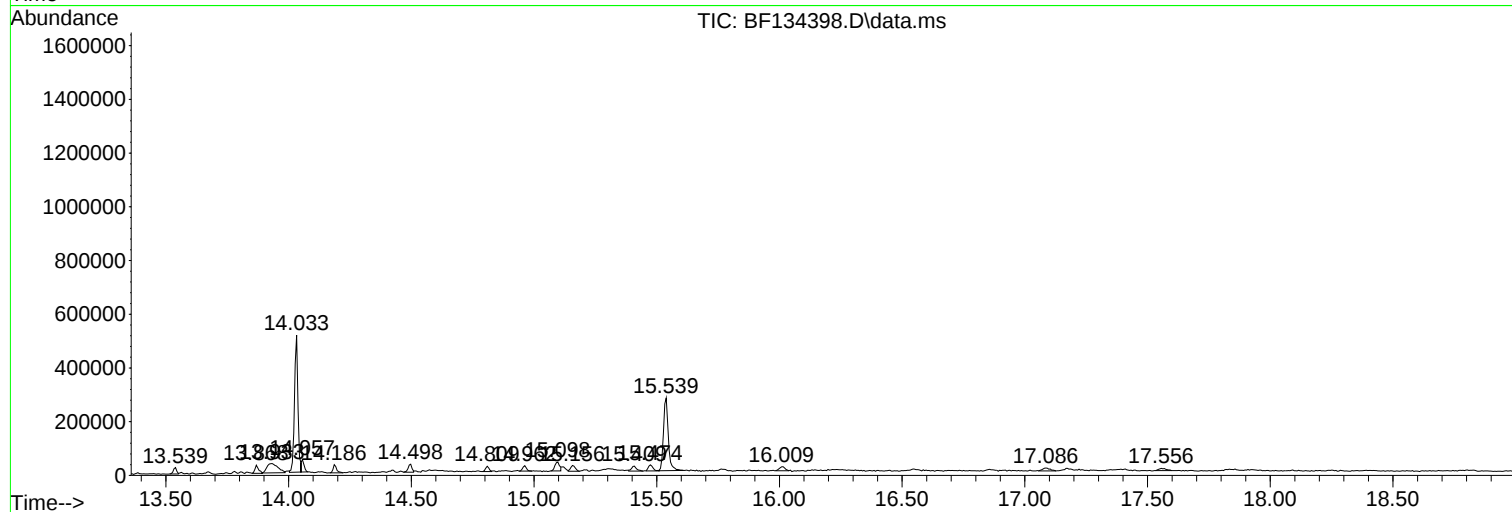
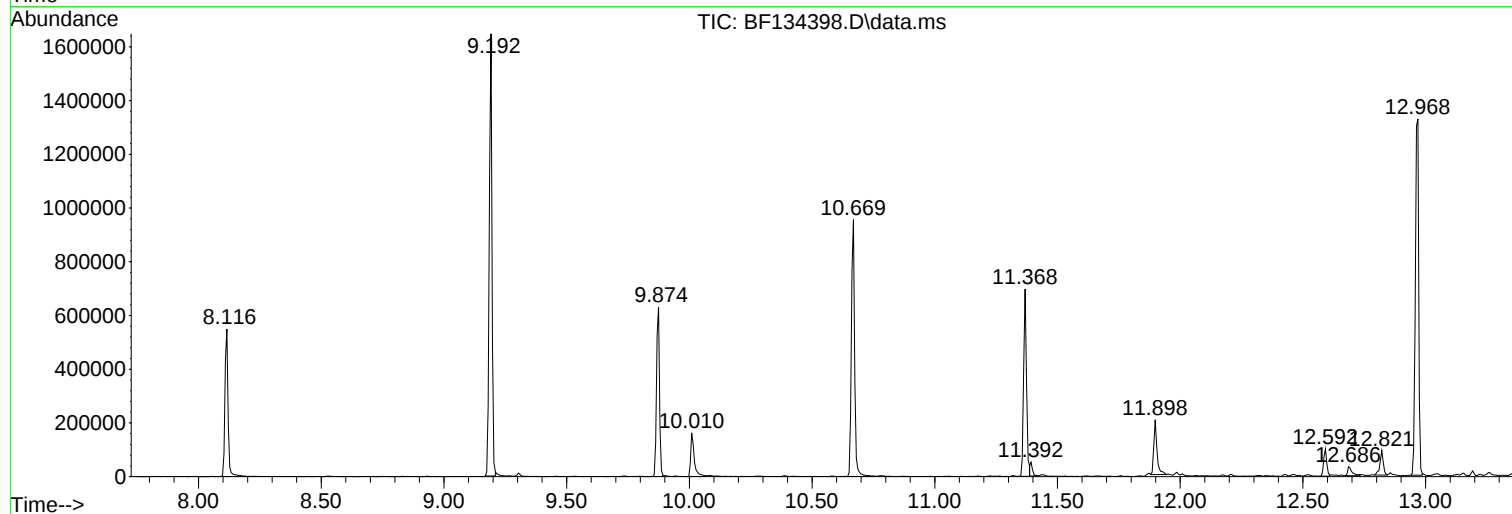
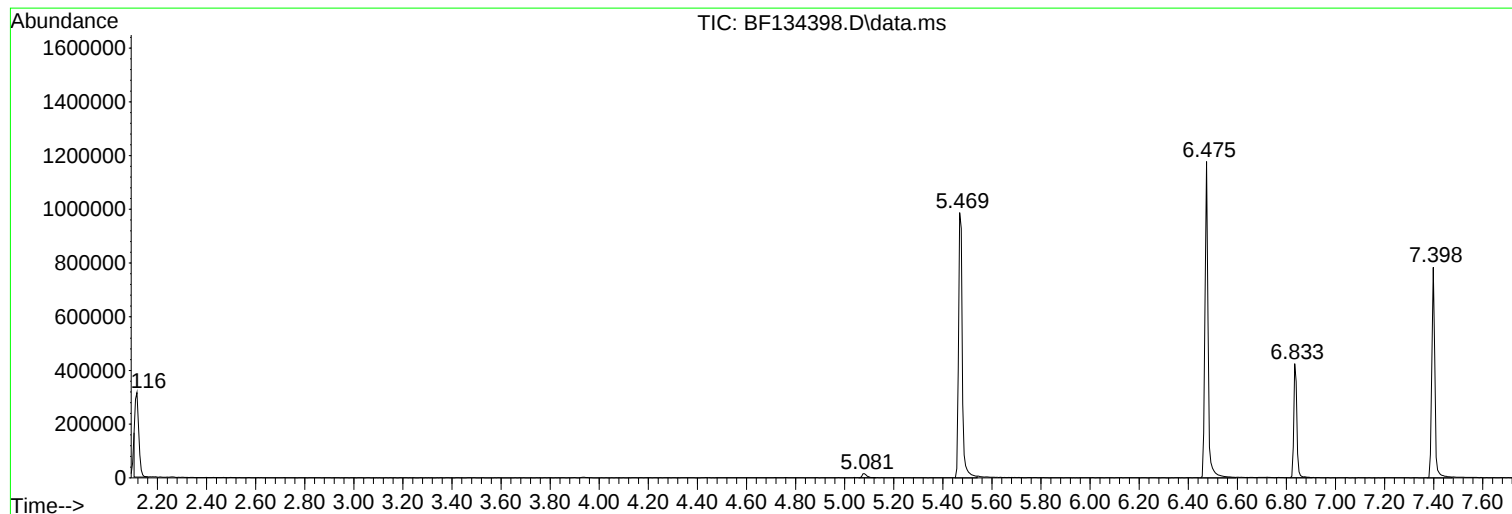
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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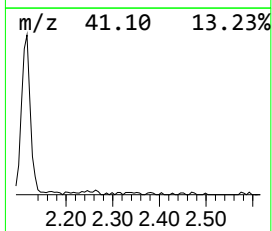
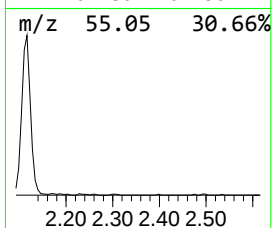
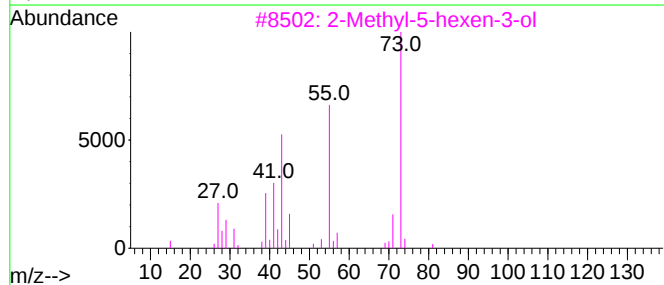
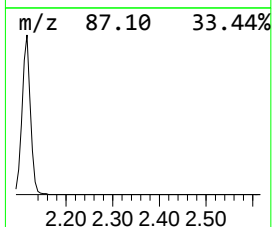
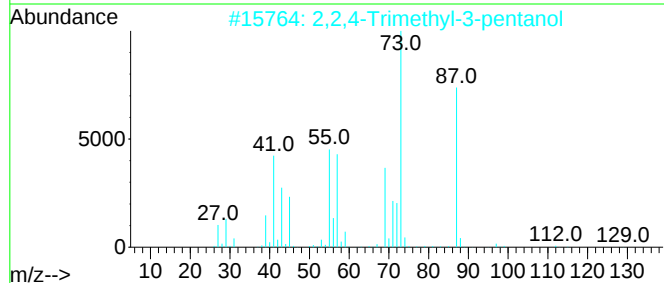
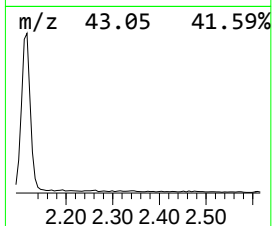
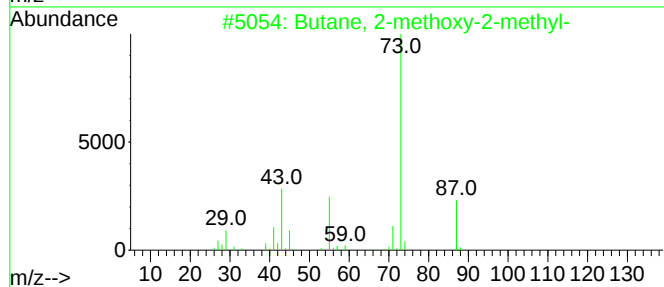
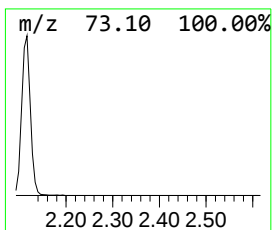
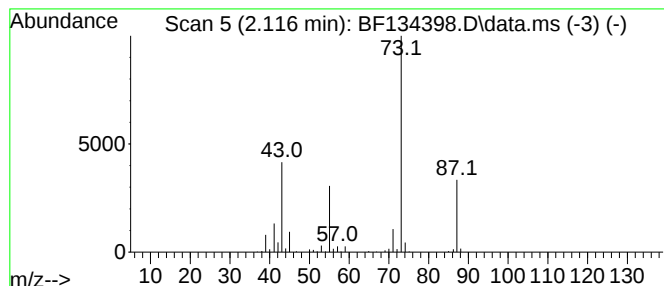
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	17.86 ng	326674	1,4-Dichlorobenzene-d4	6.833

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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25



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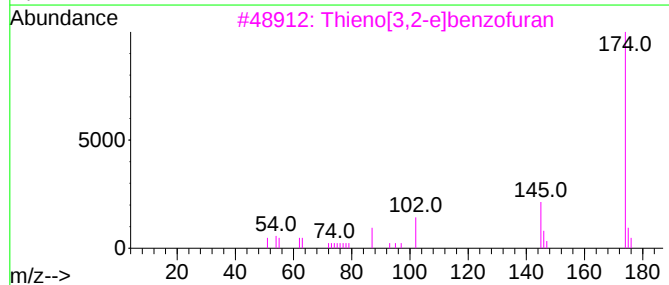
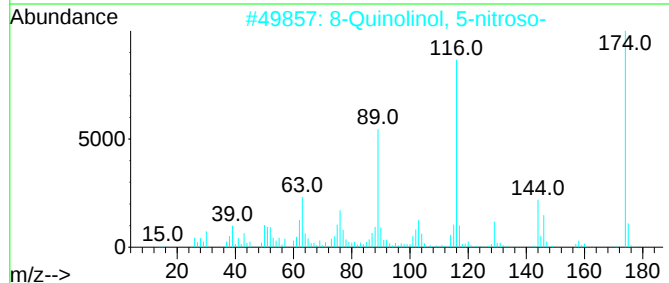
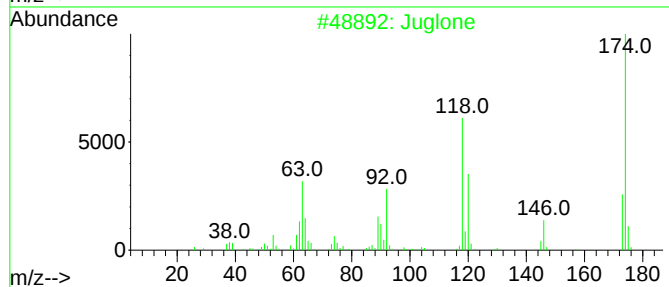
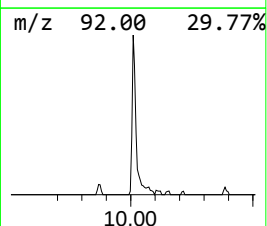
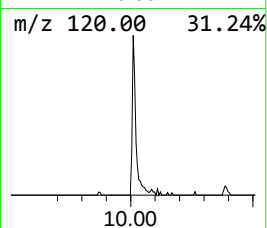
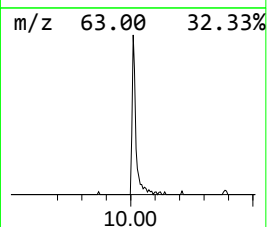
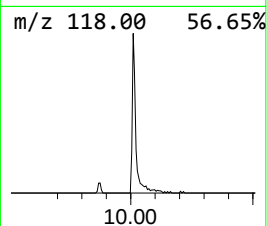
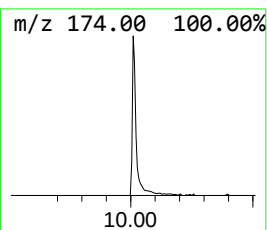
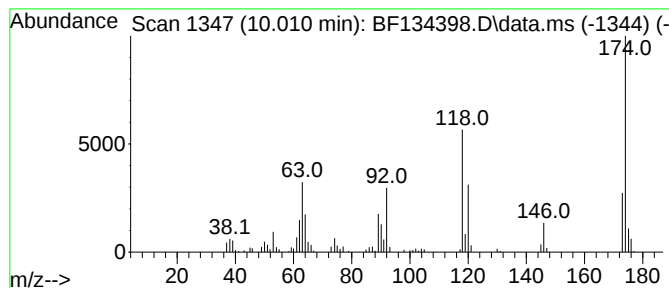
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Juglone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	6.14 ng	162802	Acenaphthene-d10	9.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Juglone	174	C10H6O3	000481-39-0	99
2			8-Quinolinol, 5-nitroso-	174	C9H6N2O2	003565-26-2	43
3			Thieno[3,2-e]benzofuran	174	C10H6O5	000438-27-7	38
4			1-(3-Pyridinylmethyl)-3-piperidi...	261	C15H23N3O	1000469-14-1	38
5			4-(3-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-18-3	35



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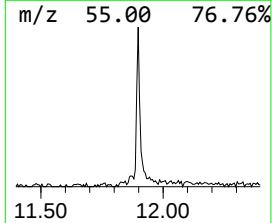
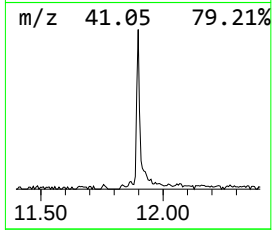
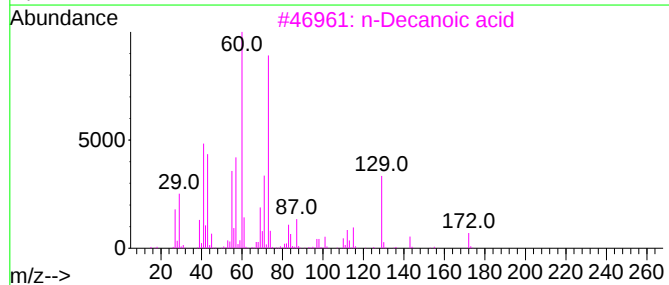
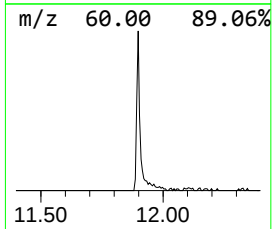
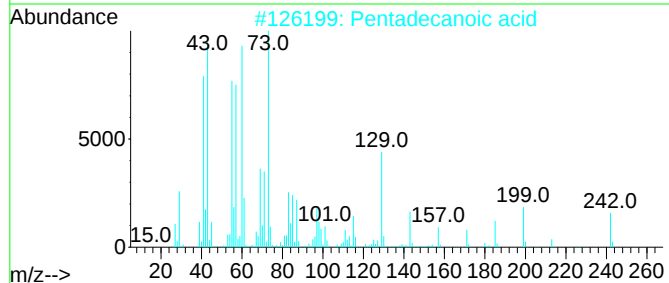
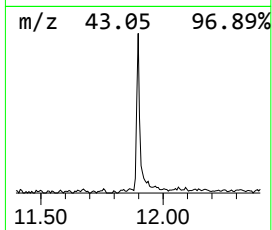
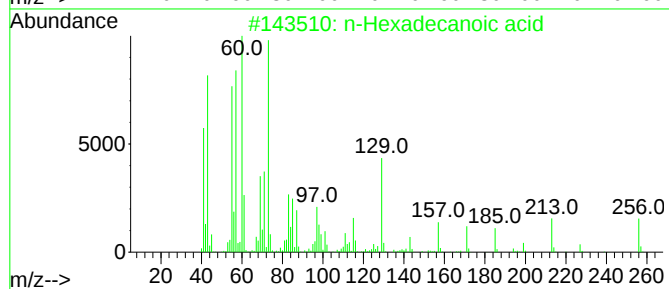
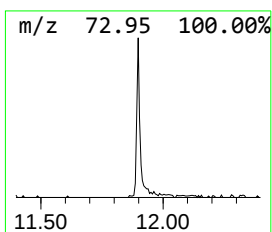
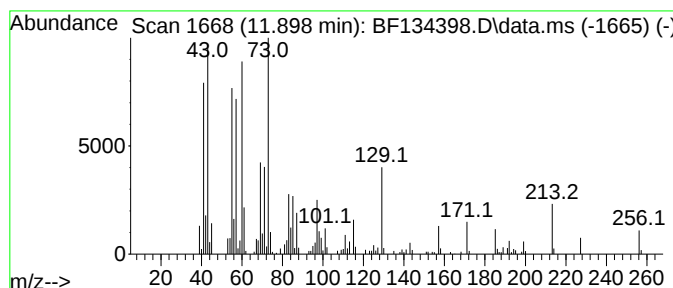
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.898	6.47 ng	184209	Phenanthrene-d10		11.368	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
3	n-Decanoic acid		172	C10H20O2	000334-48-5	76
4	Tridecanoic acid		214	C13H26O2	000638-53-9	70
5	Dodecanoic acid		200	C12H24O2	000143-07-7	58



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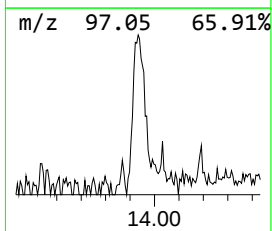
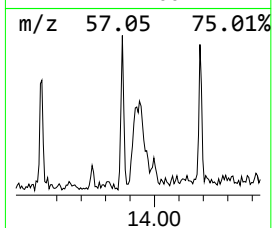
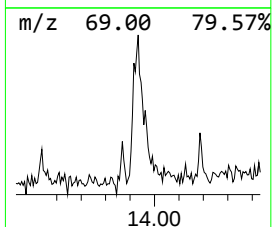
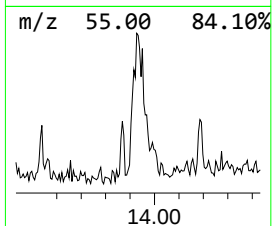
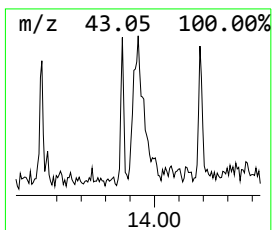
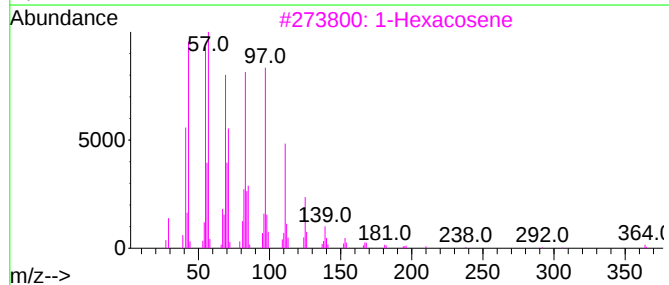
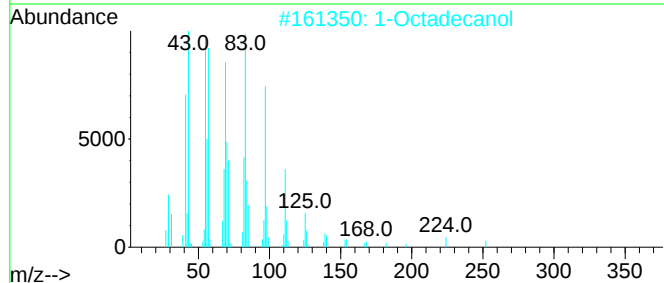
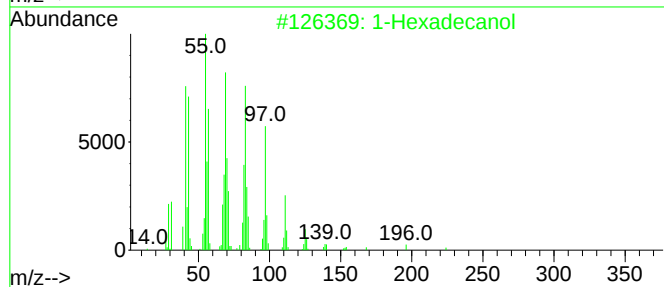
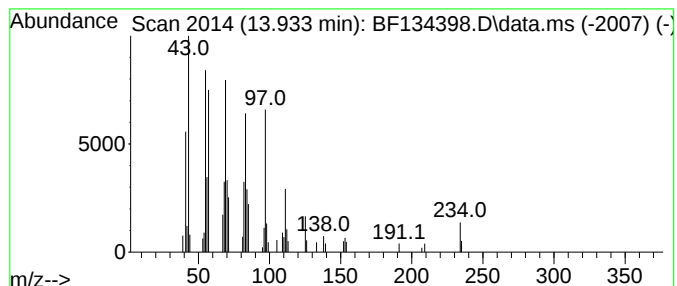
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	4.32 ng	108809	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanol	242	C16H34O	036653-82-4	90
2			1-Octadecanol	270	C18H38O	000112-92-5	90
3			1-Hexacosene	364	C26H52	018835-33-1	87
4			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	68
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	64



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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...	2.116	17.9	ng	326674	1	6.833	365830	20.0
Juglone	10.010	6.1	ng	162802	3	9.874	530592	20.0
n-Hexadecanoic ...	11.898	6.5	ng	184209	4	11.368	569067	20.0
1-Hexadecanol	13.933	4.3	ng	108809	5	14.033	503543	20.0