

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120921\
 Data File : BP008326.D
 Acq On : 09 Dec 2021 23:23
 Operator : CG/JU
 Sample : M4966-14
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 P2-COMP

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_P\Methods\8270E-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008326.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	20	rVB	178638	226680	6.49%	1.190%
2	3.969	163	167	172	rVB	27871	39271	1.12%	0.206%
3	4.522	257	261	267	rVB	25040	35862	1.03%	0.188%
4	4.893	319	324	336	rBV	160458	234294	6.71%	1.230%
5	5.363	397	404	410	rBV	1169939	1786714	51.16%	9.382%
6	5.411	410	412	425	rVB	65044	123312	3.53%	0.647%
7	5.781	469	475	481	rVB	25416	39891	1.14%	0.209%
8	6.958	665	675	687	rBV	1007598	1837727	52.62%	9.650%
9	7.763	805	812	820	rBV	263950	425371	12.18%	2.234%
10	8.928	1003	1010	1026	rBV	644141	1137180	32.56%	5.971%
11	10.563	1280	1288	1301	rBV	294678	541679	15.51%	2.844%
12	13.034	1701	1708	1732	rBV	1434217	2246356	64.32%	11.795%
13	14.328	1921	1928	1934	rBV	24633	41113	1.18%	0.216%
14	14.416	1936	1943	1956	rVV	444063	699803	20.04%	3.675%
15	15.845	2181	2186	2192	rBV	82348	110702	3.17%	0.581%
16	15.922	2192	2199	2216	rBV	1064568	1792632	51.33%	9.413%
17	17.180	2407	2413	2423	rBV	546713	870387	24.92%	4.570%
18	17.310	2431	2435	2442	rVB5	33532	54434	1.56%	0.286%
19	17.480	2460	2464	2473	rBV2	19672	35015	1.00%	0.184%
20	17.845	2522	2526	2533	rVB5	21931	46034	1.32%	0.242%
21	18.086	2562	2567	2572	rBV3	58457	90191	2.58%	0.474%
22	18.151	2574	2578	2582	rVB	32453	42627	1.22%	0.224%
23	18.980	2715	2719	2727	rVB4	25164	46301	1.33%	0.243%
24	19.210	2754	2758	2765	rVB5	33436	58371	1.67%	0.306%
25	19.757	2845	2851	2860	rBV	2810506	3492554	100.00%	18.339%
26	20.504	2975	2978	2982	rVB2	69681	72053	2.06%	0.378%
27	21.004	3059	3063	3071	rVB2	211048	326279	9.34%	1.713%
28	21.198	3093	3096	3101	rVB	138136	146666	4.20%	0.770%
29	21.292	3107	3112	3122	rBV	797244	1129344	32.34%	5.930%
30	22.174	3259	3262	3266	rVB2	93312	111673	3.20%	0.586%
31	23.674	3511	3517	3529	rVB2	570054	1204160	34.48%	6.323%

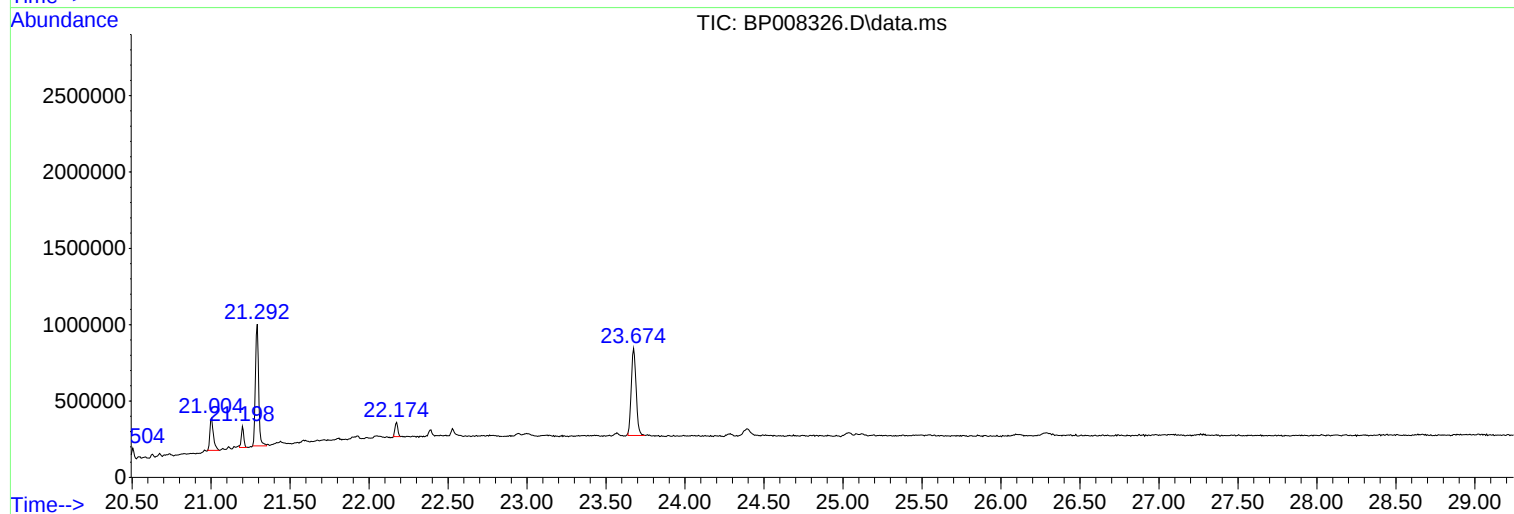
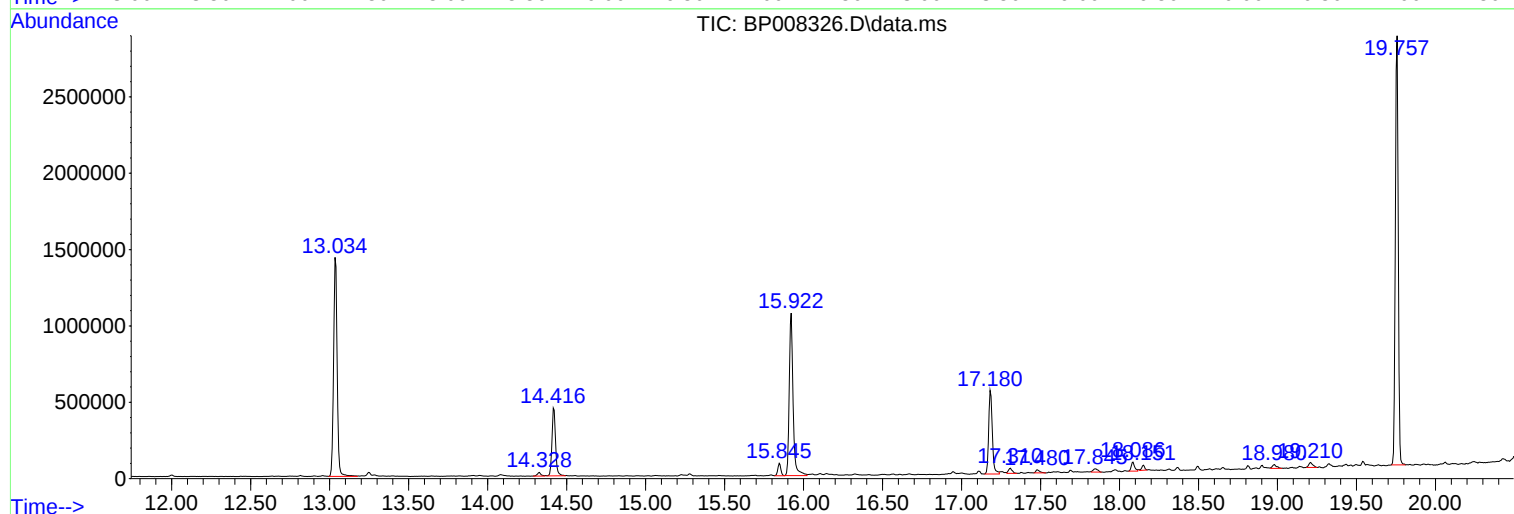
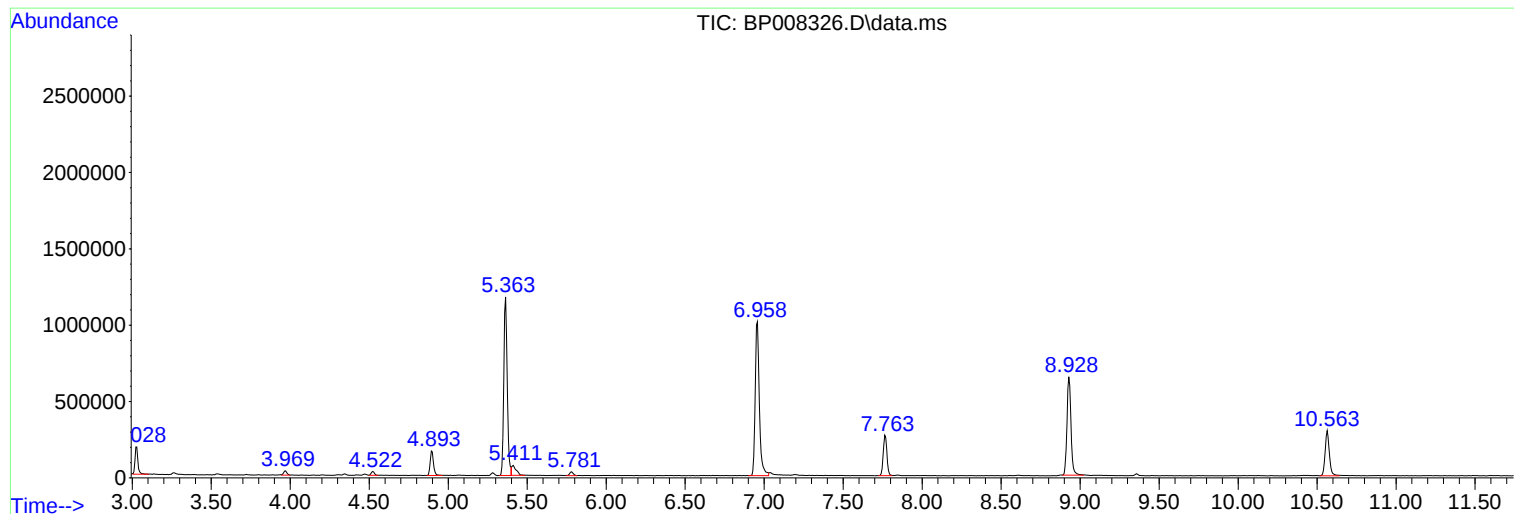
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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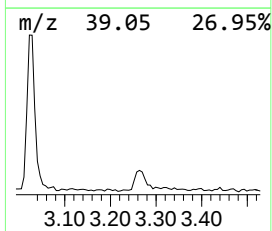
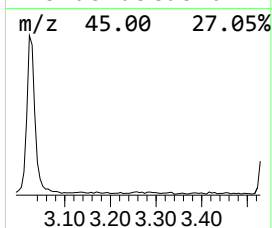
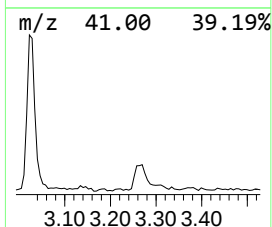
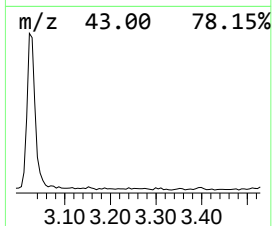
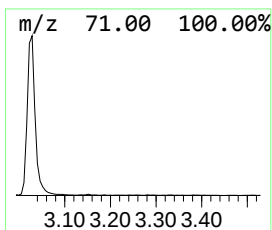
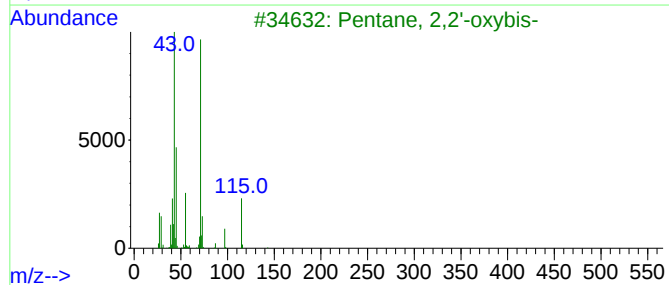
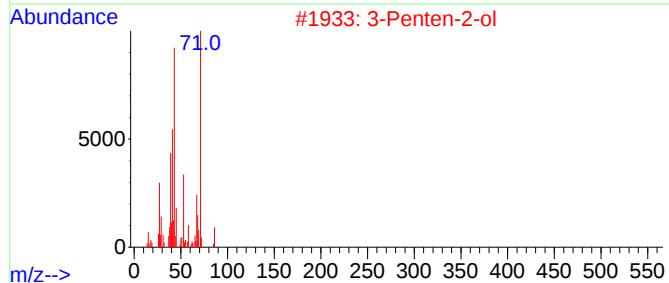
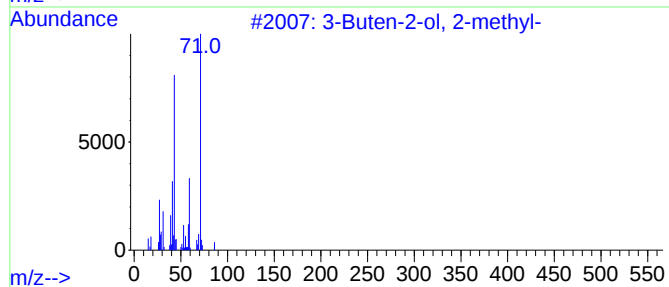
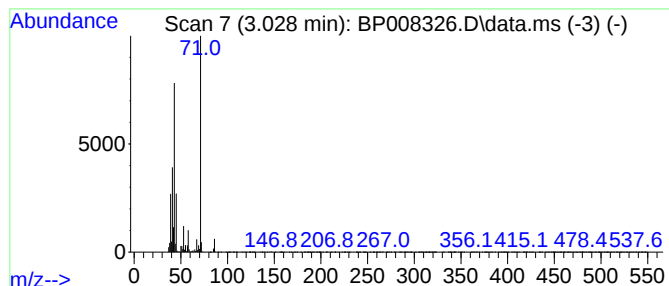
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Buten-2-ol, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	10.66 ng	226680	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
2			3-Penten-2-ol	86	C5H10O	001569-50-2	64
3			Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	64
4			Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	56
5			Pentane, 3-bromo-	150	C5H11Br	001809-10-5	53



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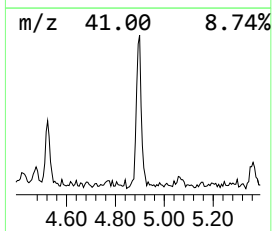
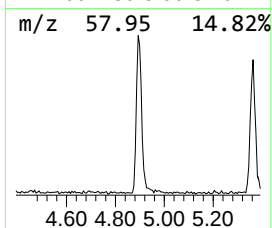
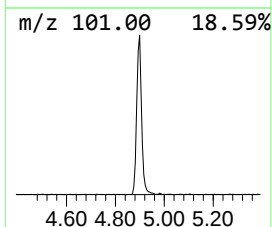
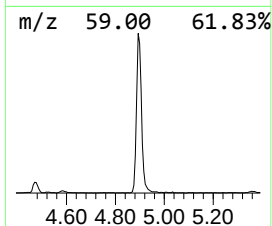
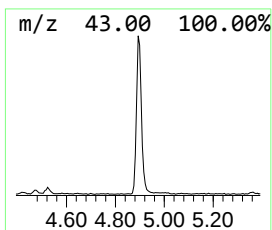
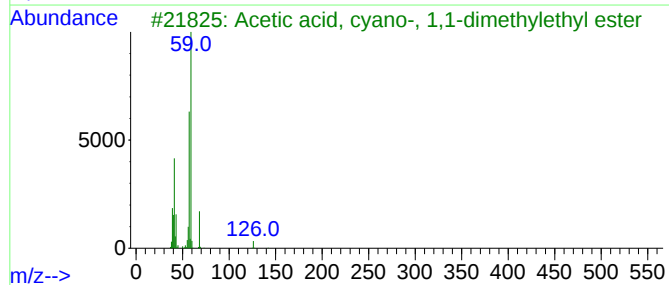
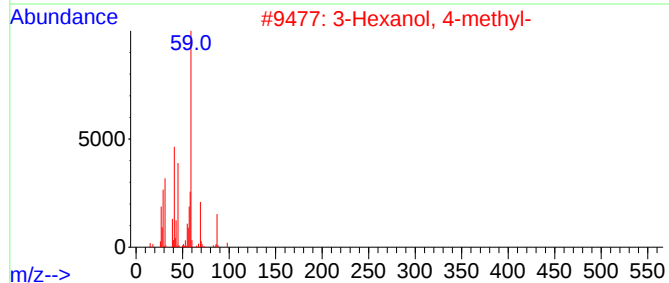
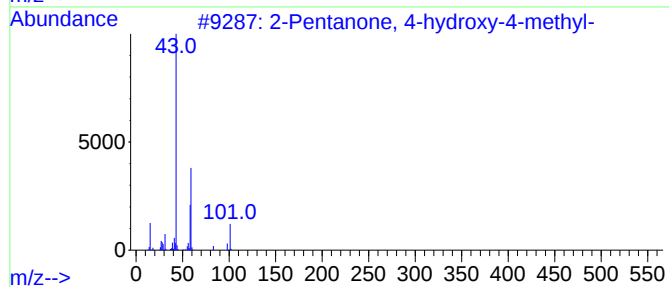
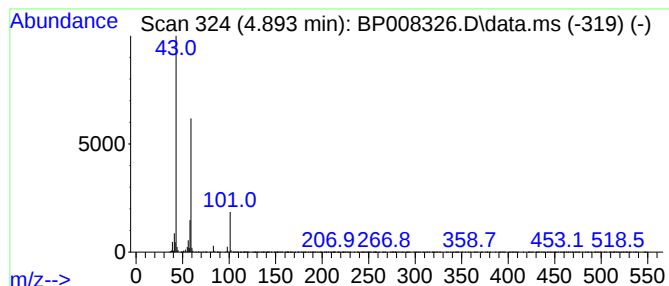
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.893	11.02 ng	234294	1,4-Dichlorobenzene-d4			7.763
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	42
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
4	Guanidine		59	CH5N3	000113-00-8	9
5	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9



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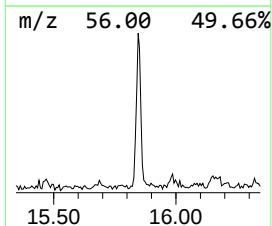
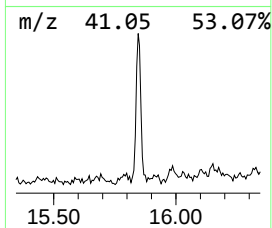
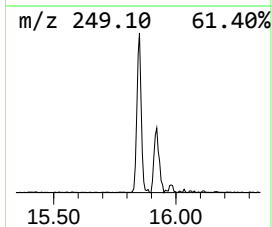
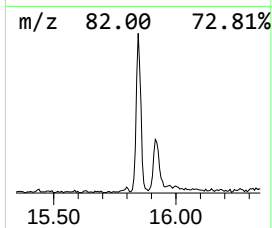
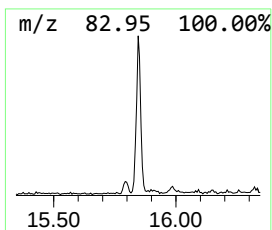
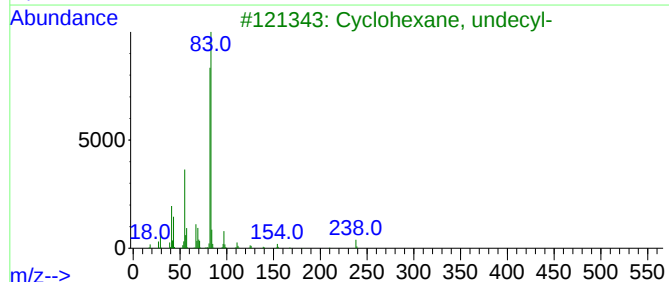
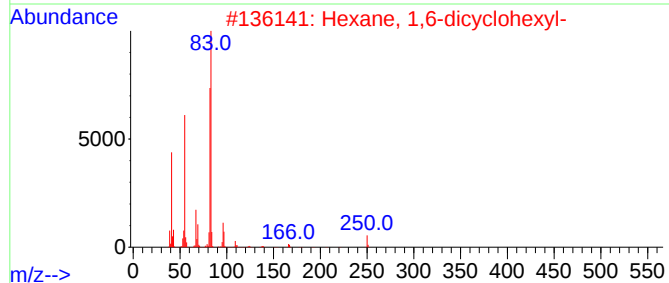
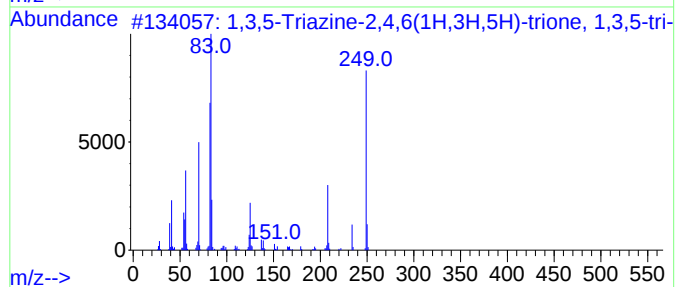
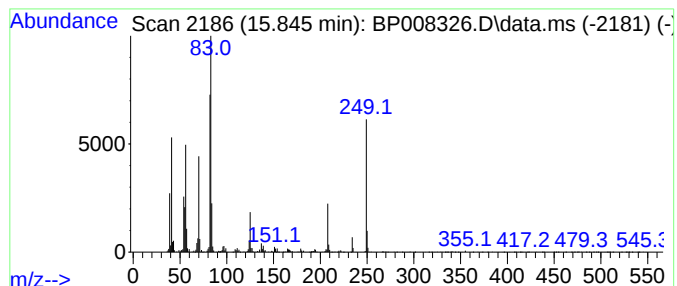
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD			R.T.
15.845	2.54 ng	110702	Phenanthrene-d10			17.180
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...		249	C12H15N3O3	001025-15-6	97
2	Hexane, 1,6-dicyclohexyl-		250	C18H34	001610-23-7	25
3	Cyclohexane, undecyl-		238	C17H34	054105-66-7	25
4	Cyclohexane, decyl-		224	C16H32	001795-16-0	16
5	Dodecylcyclohexane		252	C18H36	001795-17-1	16



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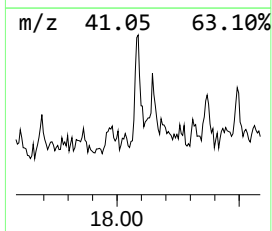
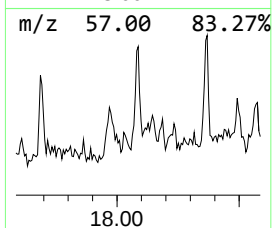
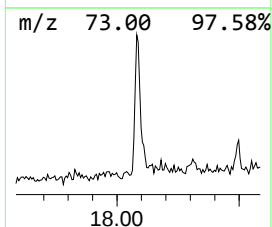
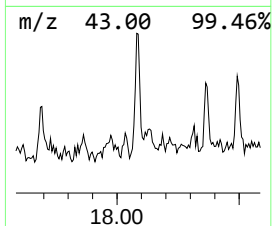
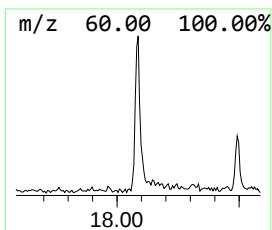
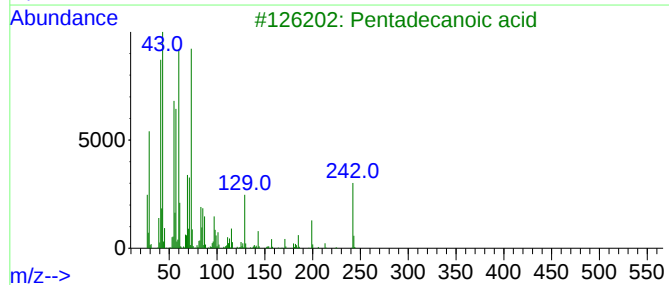
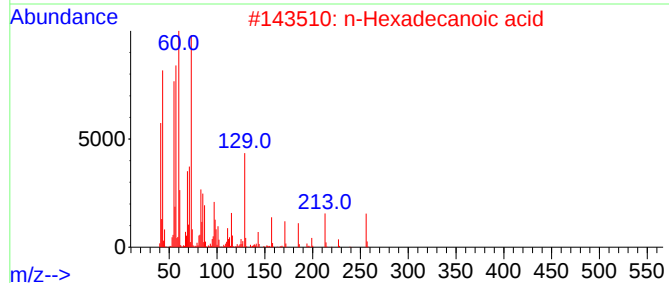
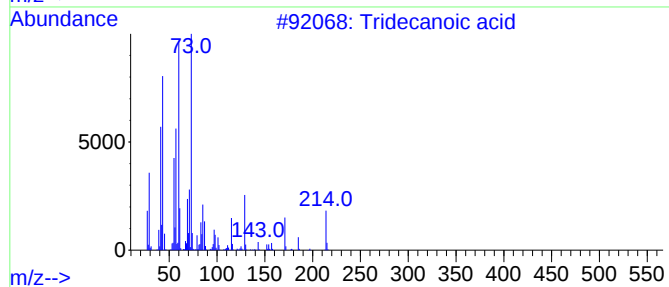
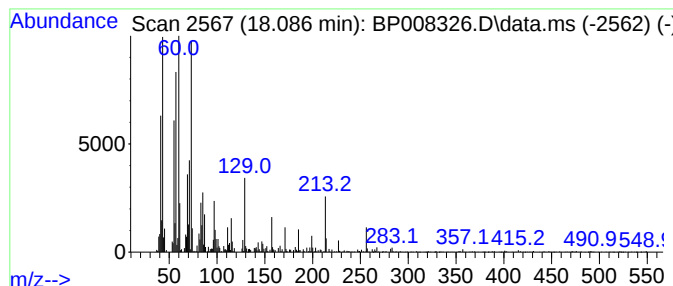
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Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.086	2.07 ng	90191	Phenanthrene-d10	17.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Dodecanoic acid	200	C12H24O2	000143-07-7	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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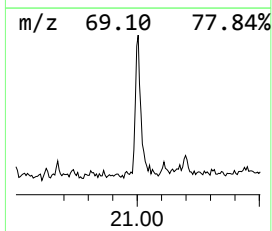
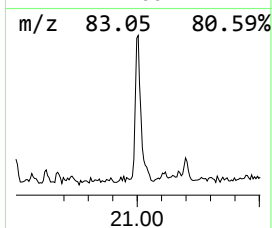
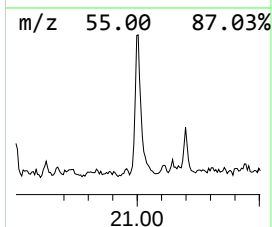
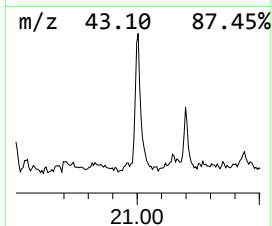
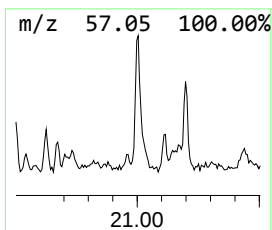
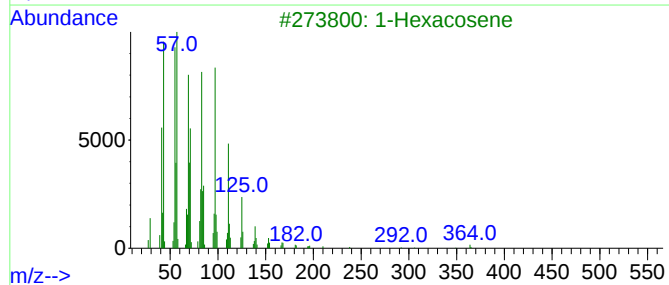
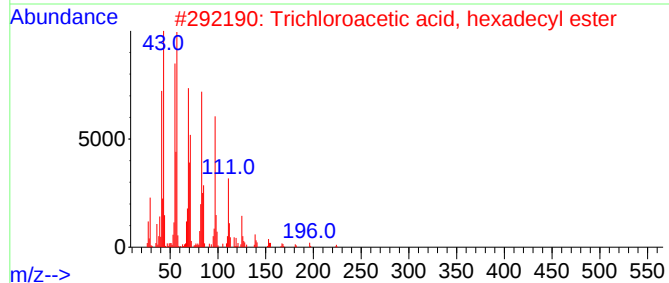
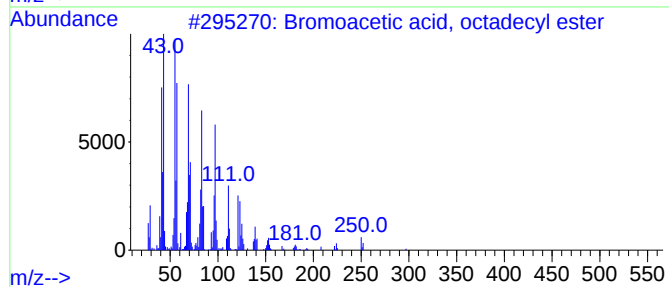
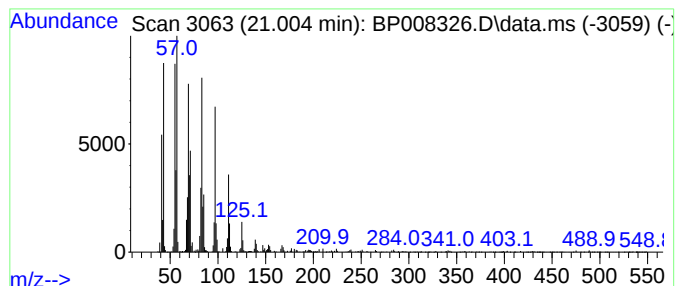
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Peak Number 5 Bromoacetic acid, octadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.004	5.78 ng	326279	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			1-Tricosene	322	C23H46	018835-32-0	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Buten-2-ol, 2...	3.028	10.7	ng	226680	1	7.763	425371	20.0
2-Pentanone, 4-...	4.893	11.0	ng	234294	1	7.763	425371	20.0
1,3,5-Triazine-...	15.845	2.5	ng	110702	4	17.180	870387	20.0
Tridecanoic acid	18.086	2.1	ng	90191	4	17.180	870387	20.0
Bromoacetic aci...	21.004	5.8	ng	326279	5	21.292	1129340	20.0