

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
 Data File : BP021521.D
 Acq On : 15 Aug 2024 20:03
 Operator : RC/JU
 Sample : P3582-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S-855-J-SO-2-2.5-081224

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-BP081324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP021521.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	24	rVB	2981264	4135685	50.19%	5.675%
2	3.540	90	94	107	rVB	204895	281835	3.42%	0.387%
3	4.934	325	331	337	rVB	175982	253219	3.07%	0.347%
4	5.393	402	409	421	rBV	3701214	5495213	66.69%	7.540%
5	6.957	667	675	689	rBV	3640560	5670150	68.82%	7.780%
6	7.798	811	818	826	rBV	1755758	2844904	34.53%	3.904%
7	8.945	1004	1013	1024	rBV	2002300	3338719	40.52%	4.581%
8	9.504	1101	1108	1116	rBV	74643	121179	1.47%	0.166%
9	10.587	1284	1292	1303	rBV	2165501	3778667	45.86%	5.185%
10	11.322	1410	1417	1427	rBV	230498	423335	5.14%	0.581%
11	13.051	1703	1711	1720	rBV	4283326	6707131	81.40%	9.203%
12	14.433	1939	1946	1953	rBV	3123401	4650886	56.45%	6.382%
13	14.675	1978	1987	1996	rBV2	91858	233449	2.83%	0.320%
14	15.945	2196	2203	2212	rBV	3155975	4682453	56.83%	6.425%
15	17.239	2417	2423	2427	rBV	3742371	5260599	63.85%	7.218%
16	17.274	2427	2429	2435	rVB	333756	426241	5.17%	0.585%
17	17.369	2441	2445	2451	rVB	87179	141554	1.72%	0.194%
18	18.186	2579	2584	2592	rBV2	430658	730624	8.87%	1.003%
19	19.368	2779	2785	2793	rBV	692784	1031389	12.52%	1.415%
20	19.510	2805	2809	2821	rBV	305540	555027	6.74%	0.762%
21	19.739	2841	2848	2856	rVB	496780	860635	10.45%	1.181%
22	19.968	2881	2887	2896	rVB	6484025	8239626	100.00%	11.306%
23	20.257	2933	2936	2942	rVB	82201	119266	1.45%	0.164%
24	20.368	2951	2955	2959	rBV	84188	113522	1.38%	0.156%
25	21.368	3121	3125	3133	rVB3	182133	325614	3.95%	0.447%
26	21.680	3171	3178	3184	rBV	2833958	4894525	59.40%	6.716%
27	21.727	3184	3186	3199	rVB	246113	412978	5.01%	0.567%
28	23.915	3551	3558	3566	rVB2	1142857	2362170	28.67%	3.241%
29	25.086	3748	3757	3766	rVB	1853276	4788178	58.11%	6.570%

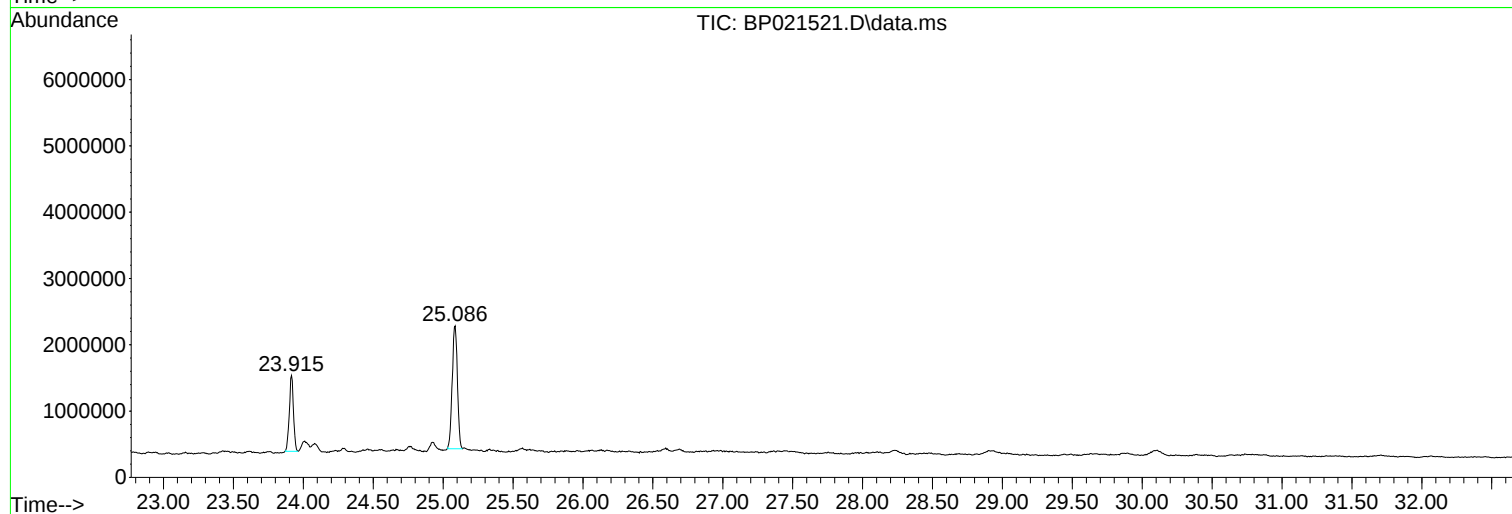
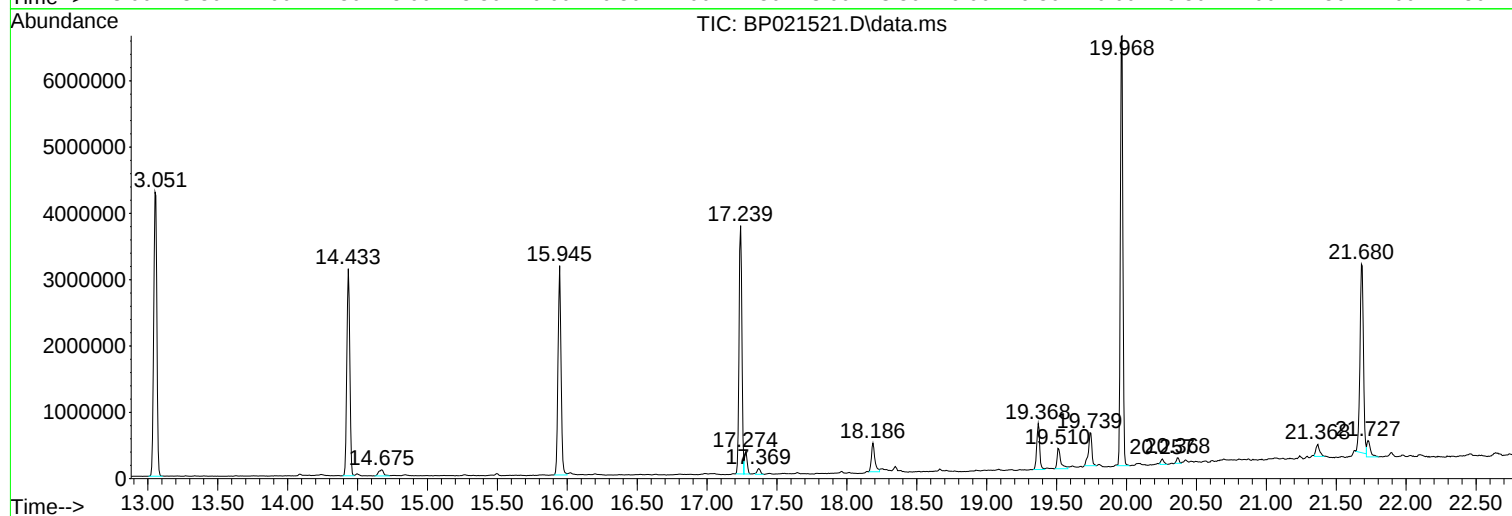
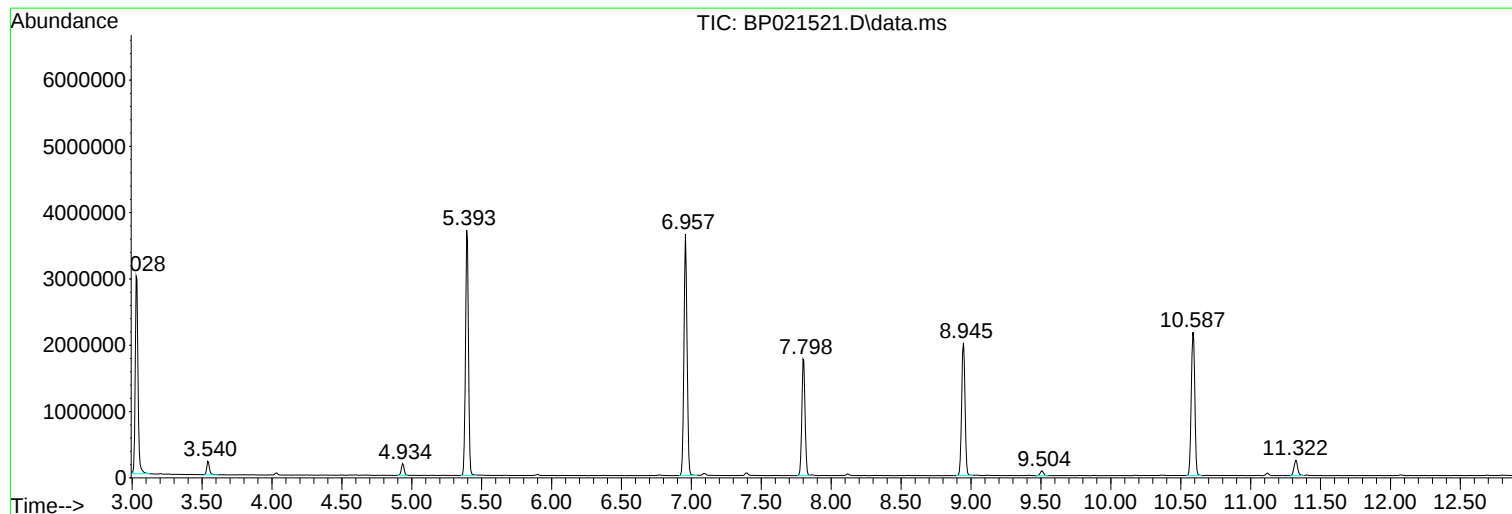
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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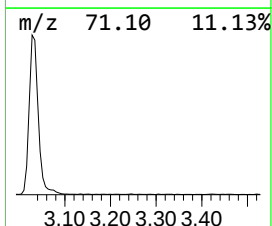
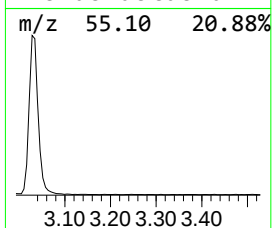
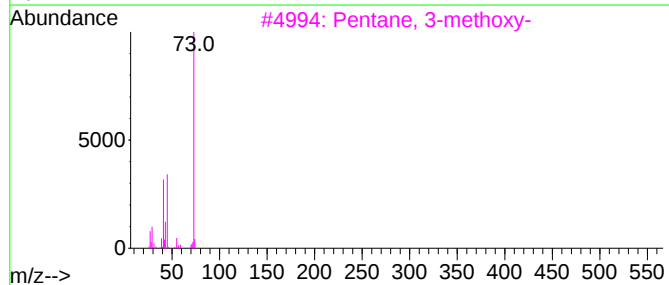
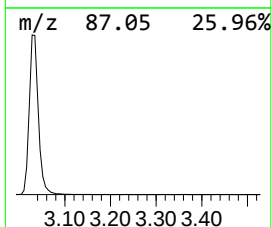
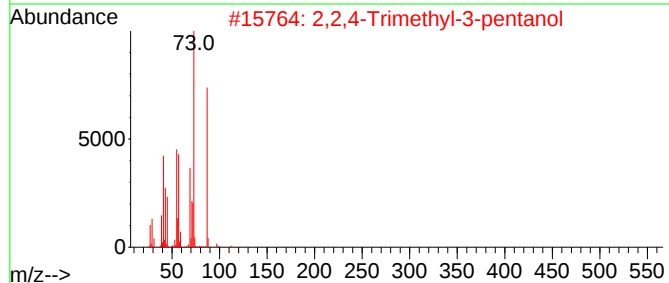
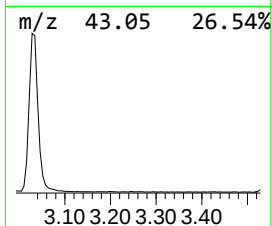
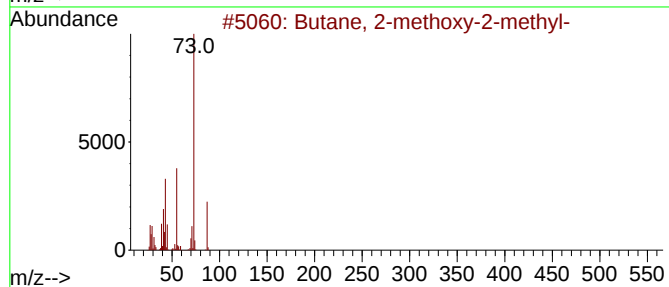
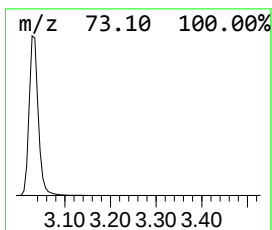
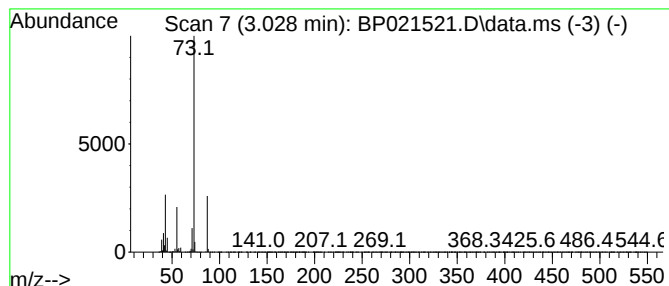
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	29.07 ng	4135690	1,4-Dichlorobenzene-d4	7.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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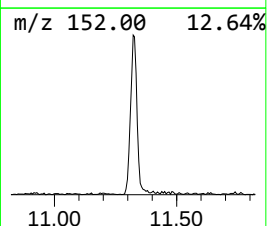
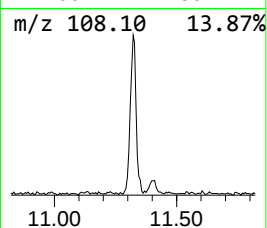
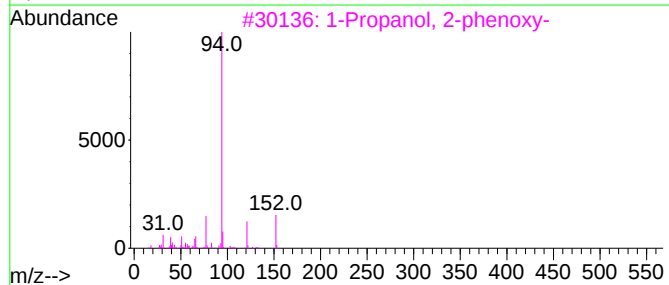
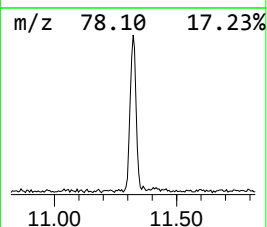
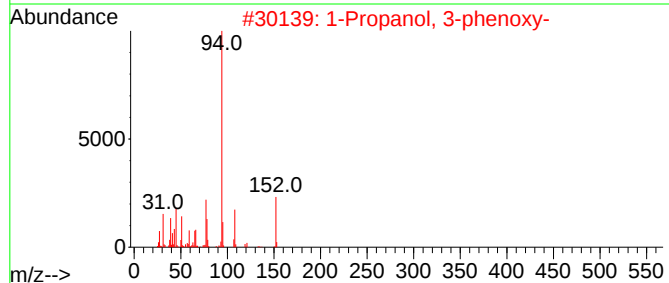
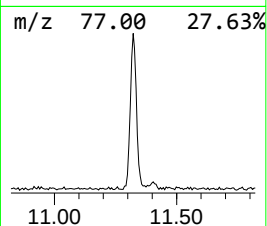
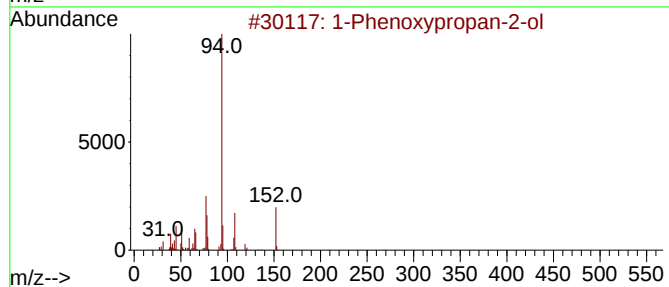
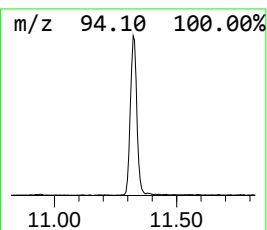
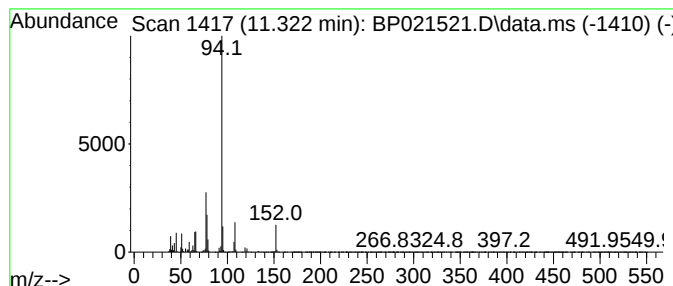
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.322	2.24 ng	423335	Naphthalene-d8	10.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4			Carbonic acid, sec-butyl phenyl ...	194	C11H14O3	013183-17-0	64
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59



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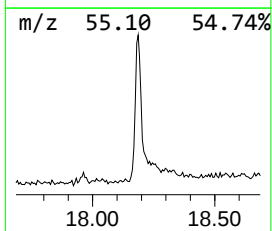
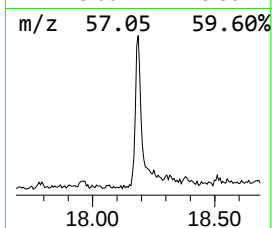
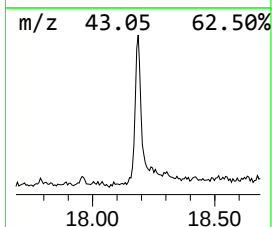
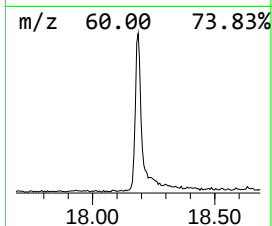
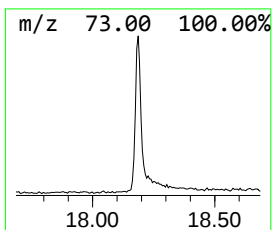
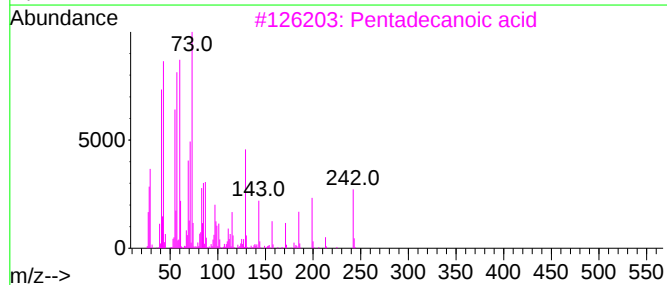
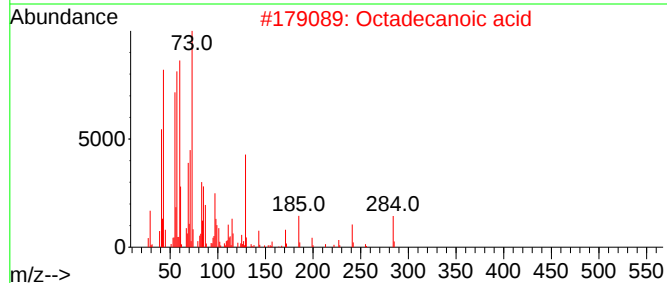
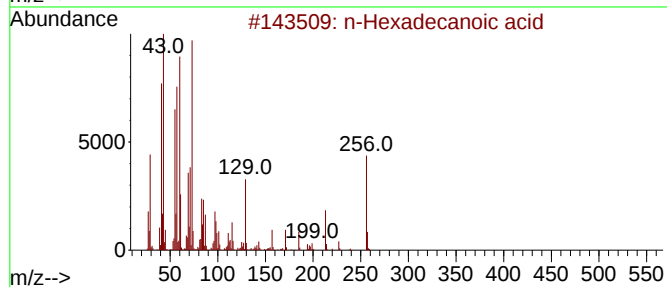
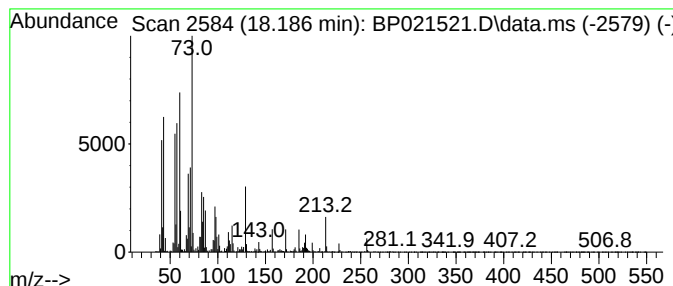
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	2.78 ng	730624	Phenanthrene-d10	17.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Octadecanoic acid	284	C18H36O2	000057-11-4	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5			n-Decanoic acid	172	C10H20O2	000334-48-5	59



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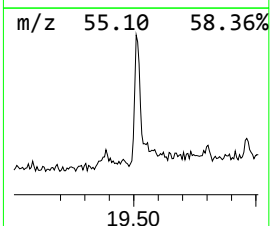
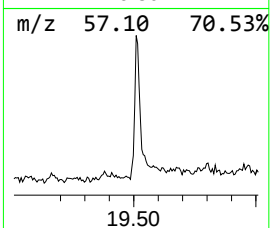
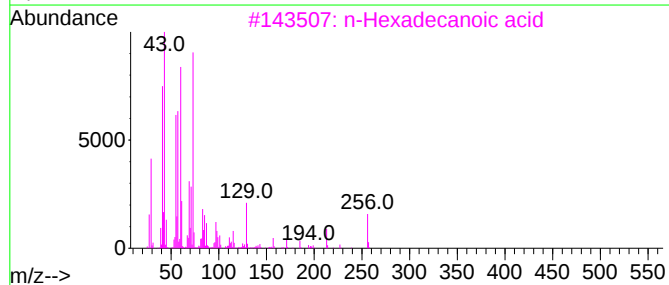
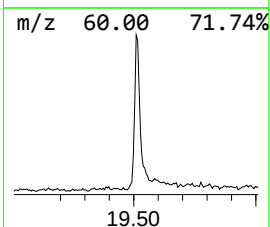
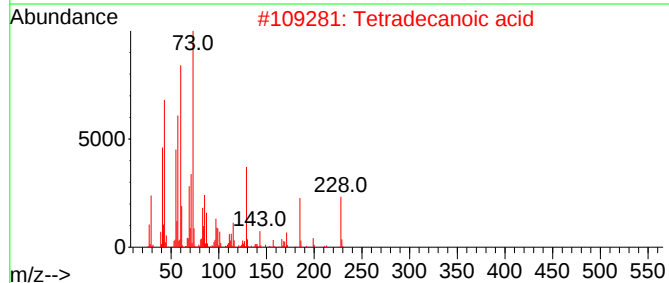
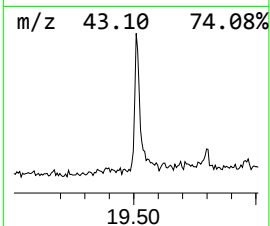
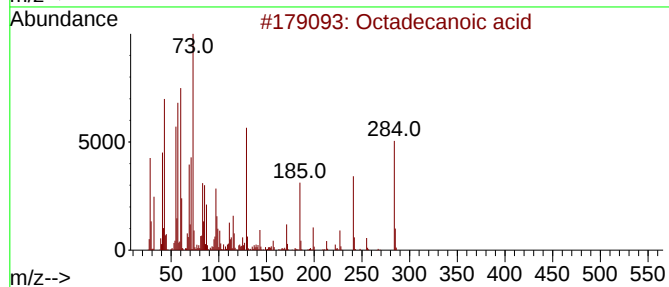
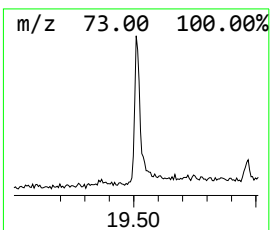
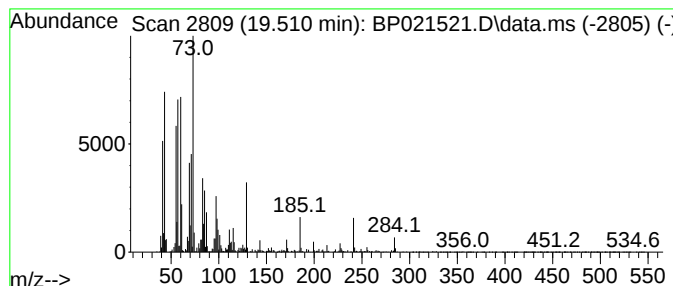
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.510	2.27 ng	555027	Chrysene-d12	21.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	47



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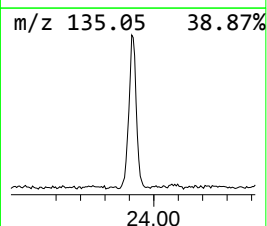
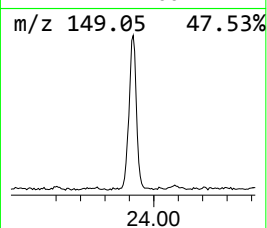
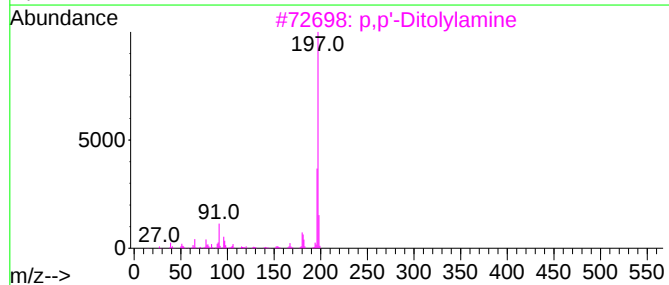
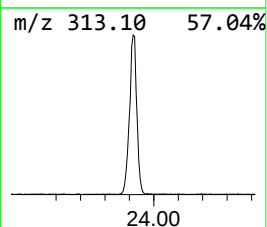
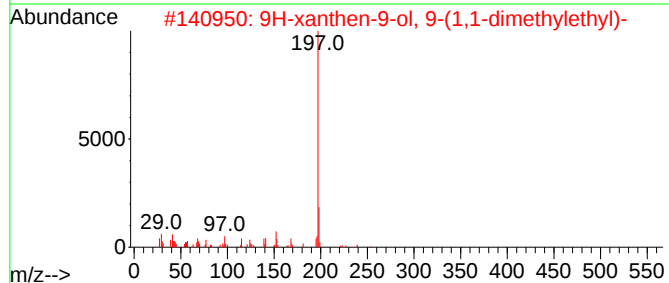
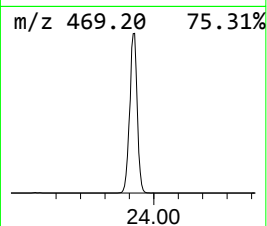
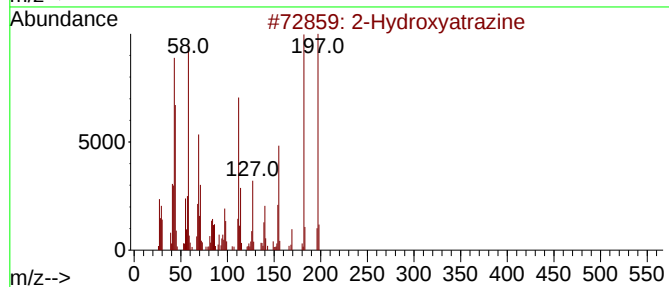
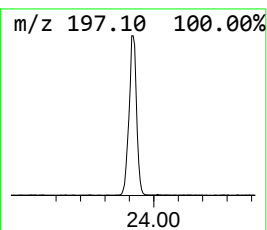
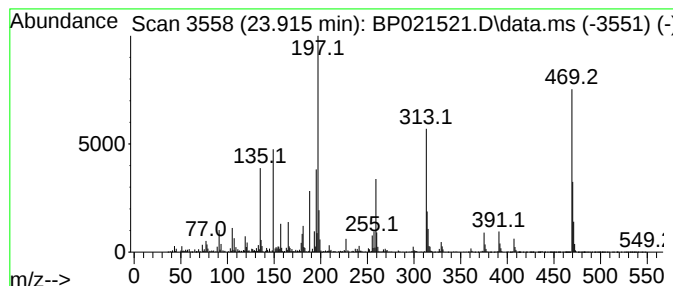
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Peak Number 5 unknown23.915 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.915	9.87 ng	2362170	Perylene-d12	25.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hydroxyatrazine	197	C8H15N5O	002163-68-0	15
2			9H-xanthen-9-ol, 9-(1,1-dimethyl...	254	C17H18O2	1000396-70-5	14
3			p,p'-Ditolylamine	197	C14H15N	000620-93-9	11
4			9H-Carbazole-3,6-diamine	197	C12H11N3	000086-71-5	11
5			3-Methoxy-4-nitrobenzyl alcohol,...	197	C9H11NO4	1000364-49-4	11



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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...	3.028	29.1	ng	4135690	1	7.804	2844900	20.0
1-Phenoxypropan...	11.322	2.2	ng	423335	2	10.587	3778670	20.0
n-Hexadecanoic ...	18.186	2.8	ng	730624	4	17.239	5260600	20.0
Octadecanoic acid	19.510	2.3	ng	555027	5	21.686	4894530	20.0
unknown23.915	23.915	9.9	ng	2362170	6	25.086	4788180	20.0