

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012723\
 Data File : BP013626.D
 Acq On : 27 Jan 2023 19:59
 Operator : CG/JU
 Sample : 01214-08
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TJRC-011723-B3-0-10-DUP

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-BP012623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.222	3	6	23	rVB	1360207	1586735	19.84%	3.250%
2	5.216	338	345	357	rBV	1226172	1759201	21.99%	3.603%
3	5.681	417	424	443	rBV	3051916	4644686	58.07%	9.512%
4	7.299	690	699	714	rBV	2872276	4742441	59.29%	9.712%
5	8.152	835	844	851	rBV	797404	1249336	15.62%	2.559%
6	9.328	1036	1044	1054	rBV	1574614	2518454	31.49%	5.158%
7	10.981	1315	1325	1333	rBV	984361	1648486	20.61%	3.376%
8	13.416	1731	1739	1753	rBV	4491842	6722228	84.04%	13.767%
9	14.787	1966	1972	1980	rBV	1395801	2019256	25.24%	4.135%
10	16.145	2195	2203	2211	rBV2	94594	161314	2.02%	0.330%
11	16.275	2218	2225	2240	rBV	3052103	4419188	55.25%	9.050%
12	17.545	2434	2441	2446	rBV	1544245	2264818	28.31%	4.638%
13	18.398	2581	2586	2592	rBV	347773	505931	6.33%	1.036%
14	19.533	2776	2779	2784	rVB	116685	147750	1.85%	0.303%
15	19.622	2790	2794	2802	rBV	157907	241116	3.01%	0.494%
16	19.886	2835	2839	2846	rVB	164505	209761	2.62%	0.430%
17	20.074	2866	2871	2880	rVB	6653244	7998726	100.00%	16.381%
18	20.363	2917	2920	2924	rVB2	103712	111235	1.39%	0.228%
19	20.739	2981	2984	2991	rBV2	116140	228026	2.85%	0.467%
20	20.845	2999	3002	3005	rVB2	114255	115149	1.44%	0.236%
21	21.298	3075	3079	3084	rBV	423791	573953	7.18%	1.175%
22	21.621	3129	3134	3139	rBV	1717900	2397750	29.98%	4.910%
23	24.210	3568	3574	3584	rVB2	1187783	2564111	32.06%	5.251%

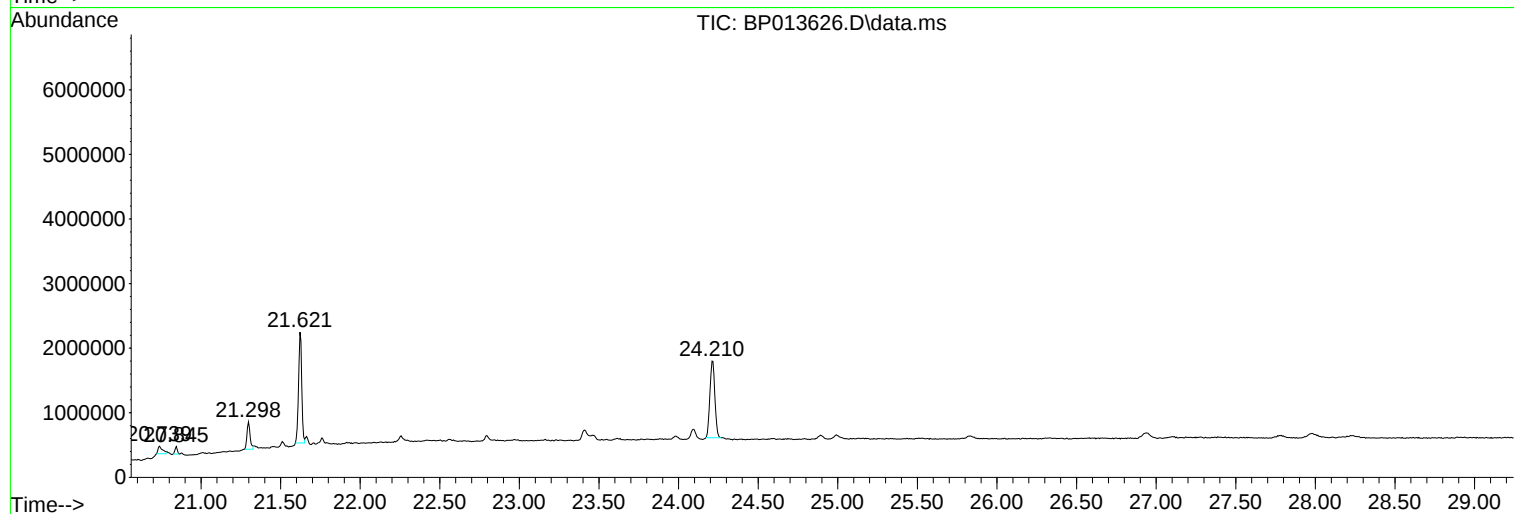
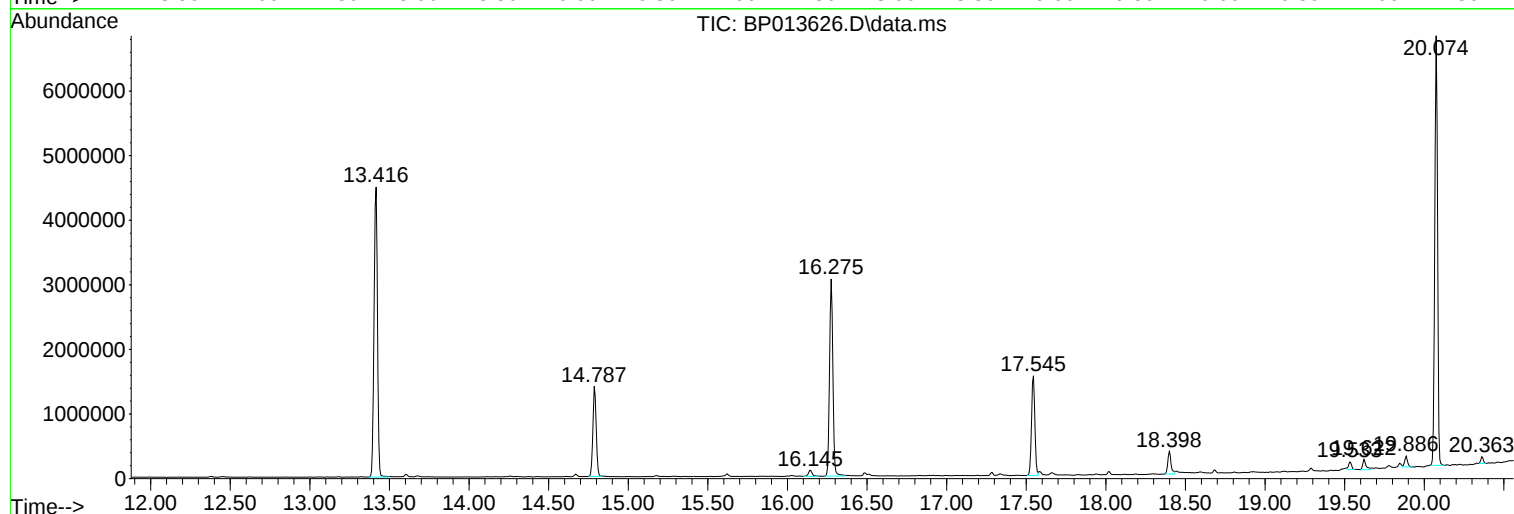
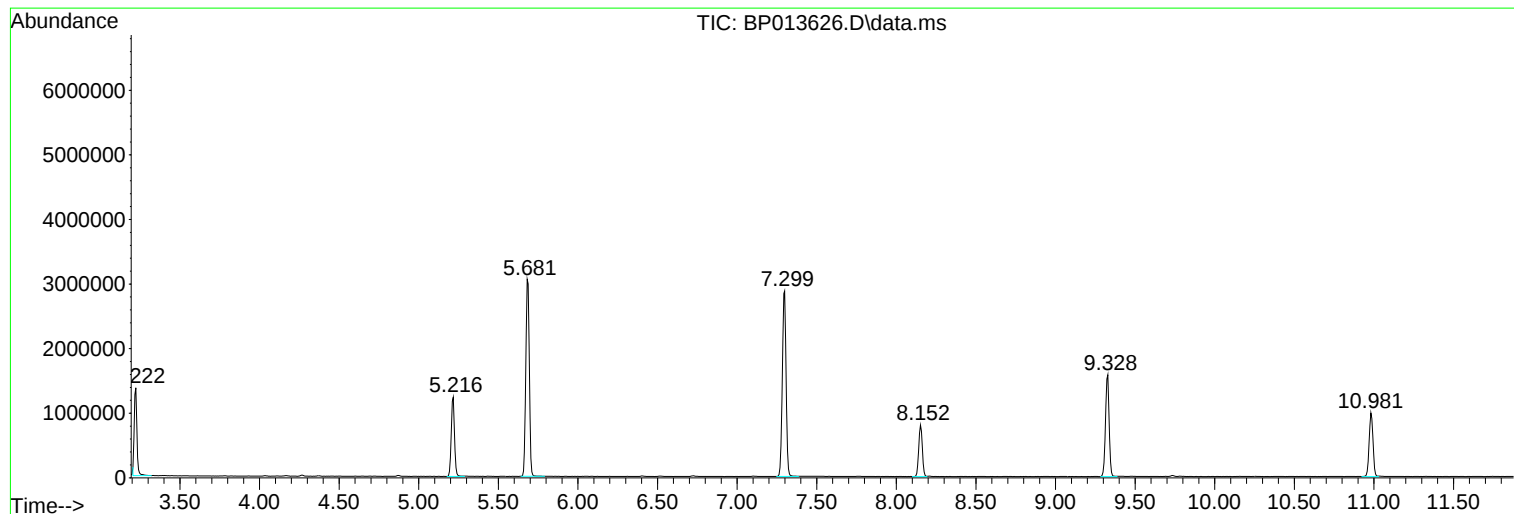
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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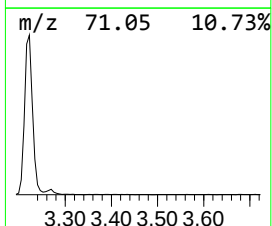
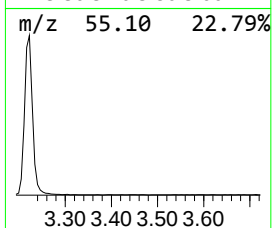
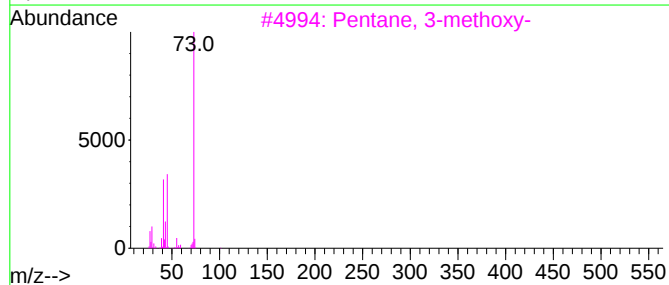
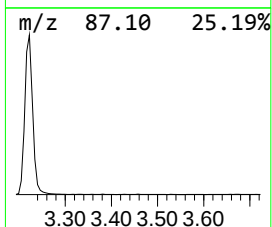
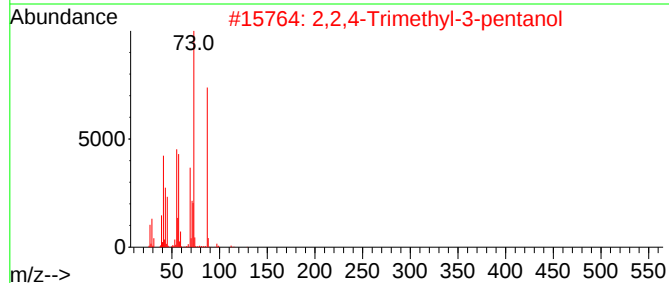
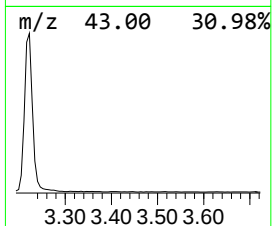
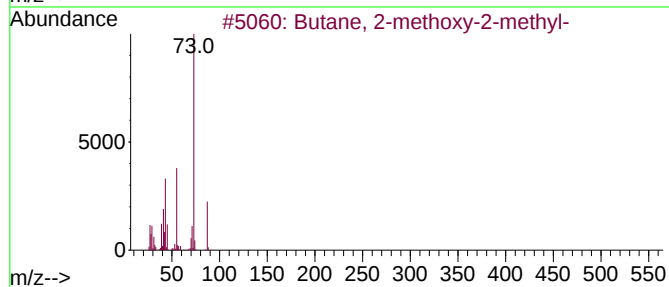
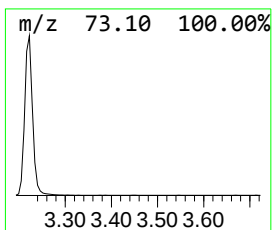
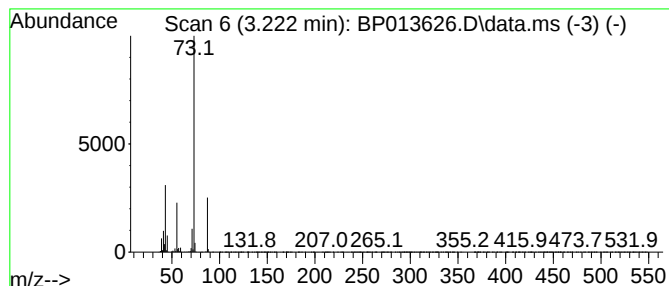
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.222	25.40 ng	1586740	1,4-Dichlorobenzene-d4	8.152

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	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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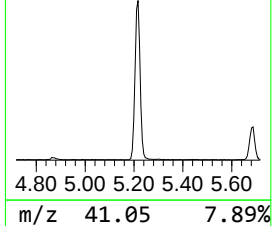
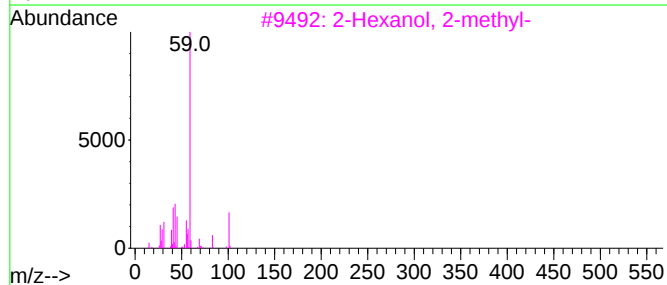
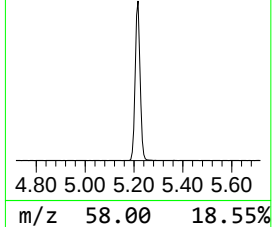
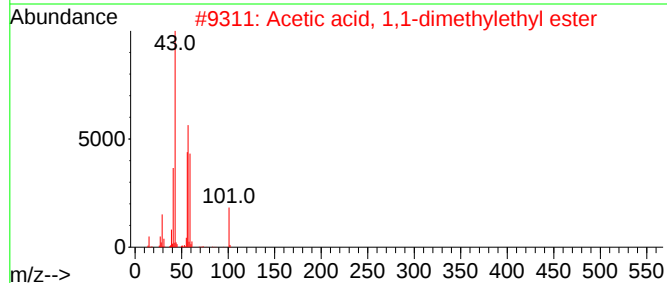
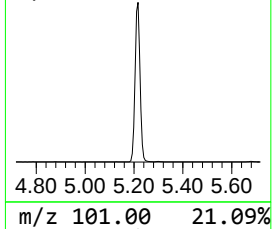
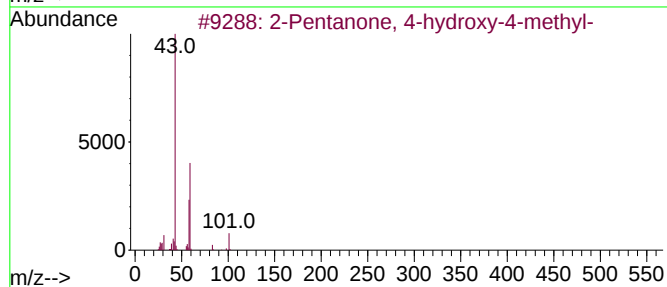
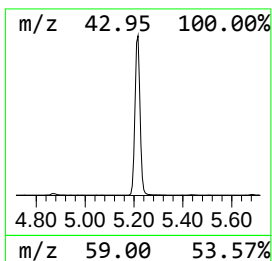
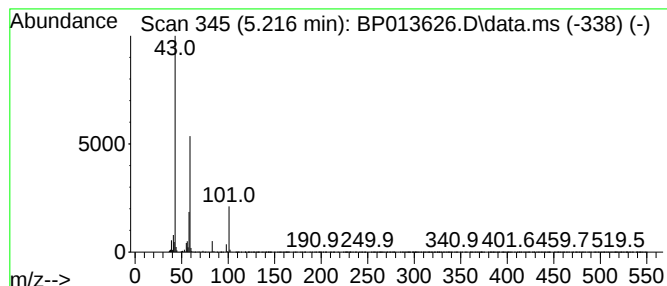
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.216	28.16 ng	1759200	1,4-Dichlorobenzene-d4			8.152
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	38
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	25
4	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	25
5	Butane, 1-ethoxy-		102	C6H14O	000628-81-9	9



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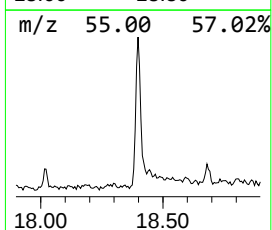
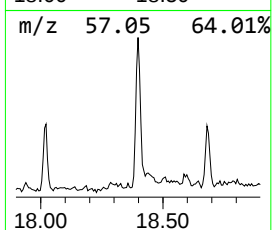
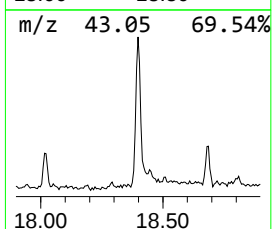
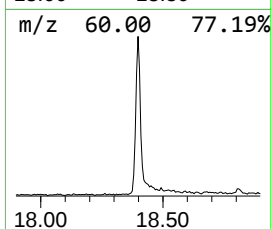
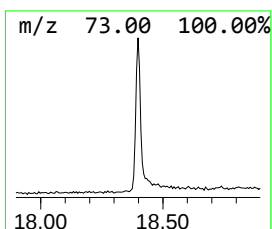
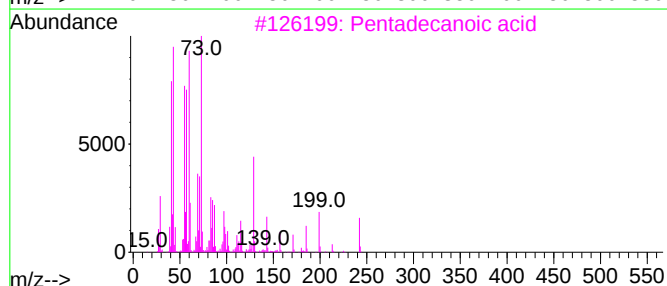
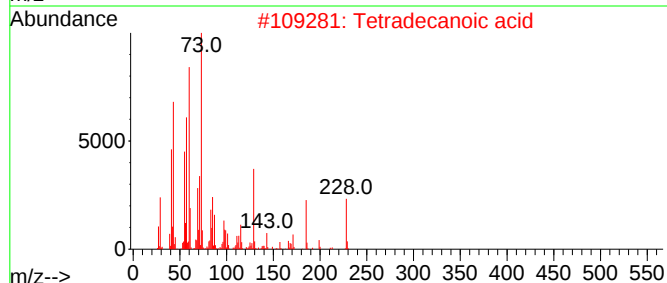
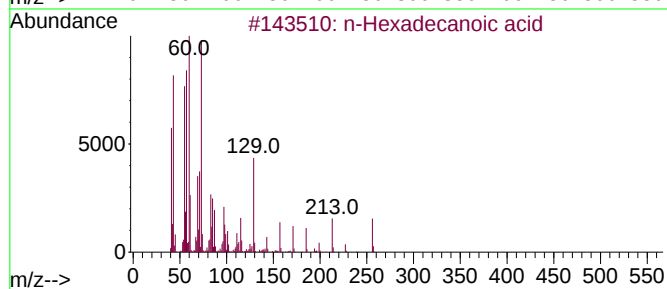
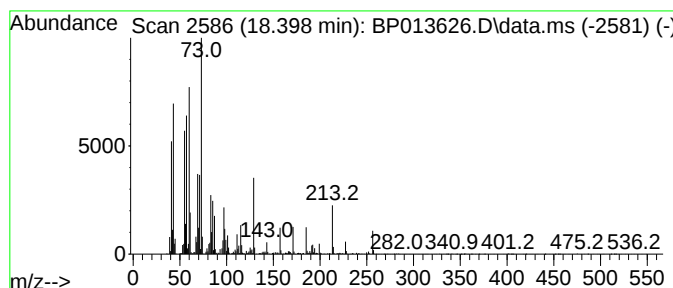
Instrument :
BNA_P
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.398	4.47 ng	505931	Phenanthrene-d10	17.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76



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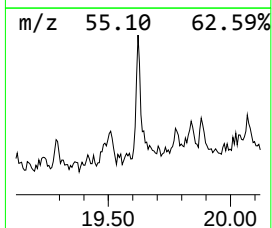
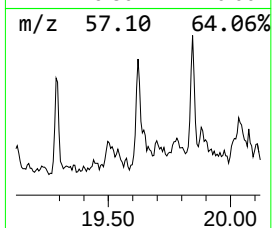
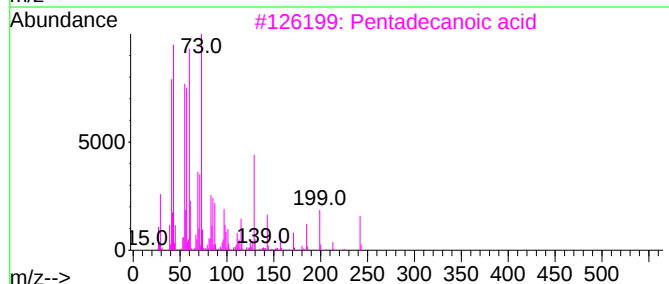
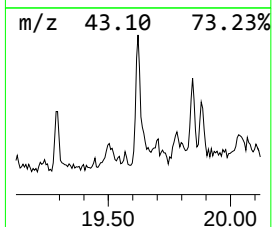
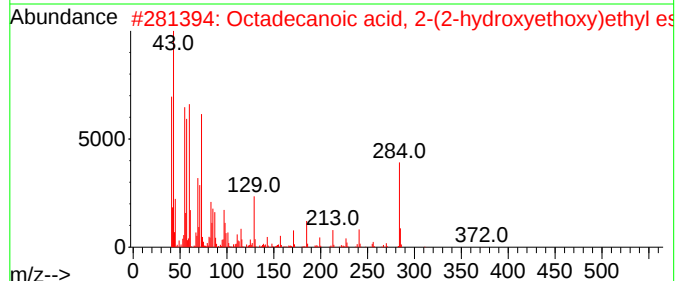
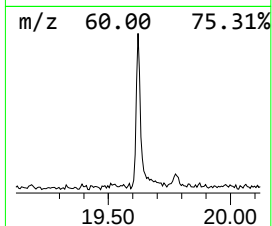
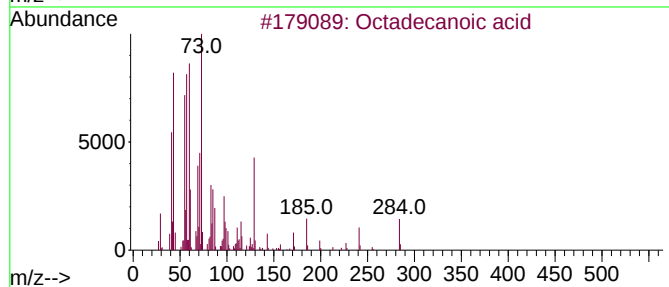
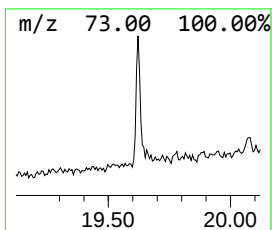
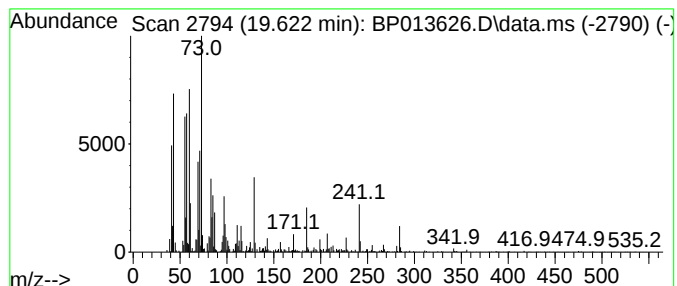
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.622	2.01 ng	241116	Chrysene-d12	21.621

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		Tridecanoic acid	214	C13H26O2	000638-53-9	52



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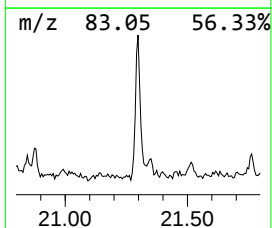
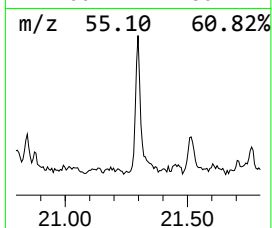
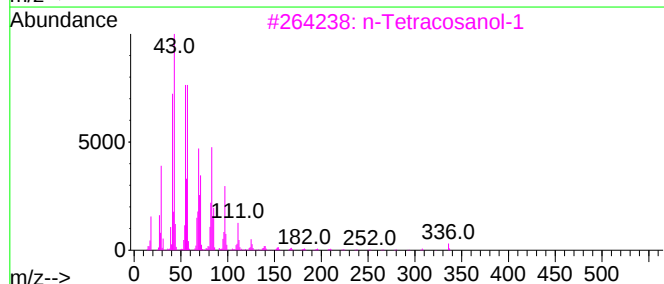
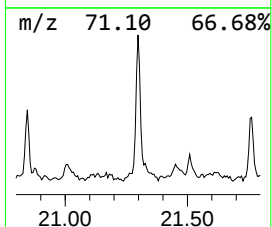
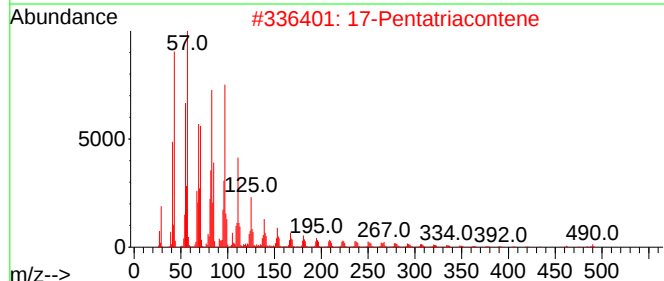
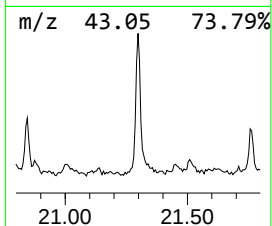
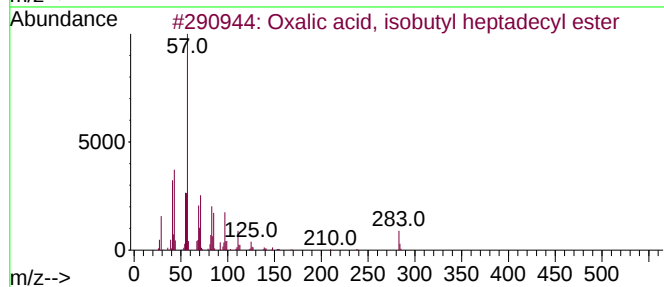
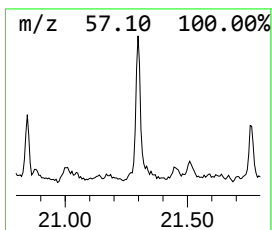
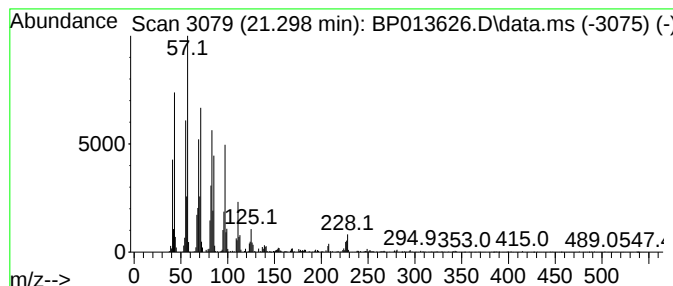
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Oxalic acid, isobutyl hepta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.298	4.79 ng	573953	Chrysene-d12	21.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87
2			17-Pentatriacontene	491	C35H70	006971-40-0	87
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	76
4			1-Hexacosanol	382	C26H54O	000506-52-5	76
5			1-Heneicosanol	312	C21H44O	015594-90-8	70



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.222	25.4	ng	1586740	1	8.152	1249340	20.0
2-Pentanone, 4-...	5.216	28.2	ng	1759200	1	8.152	1249340	20.0
n-Hexadecanoic ...	18.398	4.5	ng	505931	4	17.545	2264820	20.0
Octadecanoic acid	19.622	2.0	ng	241116	5	21.621	2397750	20.0
Oxalic acid, is...	21.298	4.8	ng	573953	5	21.621	2397750	20.0