

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012723\
 Data File : BP013629.D
 Acq On : 27 Jan 2023 21:41
 Operator : CG/JU
 Sample : 01214-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TJRC-011823-B3-20-30

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: BP013629.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	18	rVB	1259941	1459147	19.21%	2.915%
2	5.216	335	345	357	rBV	1155534	1691748	22.27%	3.380%
3	5.681	416	424	436	rBV	3016968	4546460	59.85%	9.083%
4	7.293	690	698	714	rBV	2808421	4586536	60.38%	9.163%
5	8.152	836	844	851	rBV	857869	1346676	17.73%	2.690%
6	9.322	1036	1043	1052	rBV	1455292	2348756	30.92%	4.692%
7	10.981	1313	1325	1336	rBV	1039744	1789030	23.55%	3.574%
8	12.381	1557	1563	1569	rVB	59344	85864	1.13%	0.172%
9	13.416	1731	1739	1748	rBV	4286194	6229216	82.01%	12.444%
10	13.604	1766	1771	1778	rVB	85359	118188	1.56%	0.236%
11	14.669	1947	1952	1960	rBV	122183	154789	2.04%	0.309%
12	14.786	1966	1972	1981	rVB	1457299	2197796	28.93%	4.391%
13	15.622	2110	2114	2120	rVB	161217	190384	2.51%	0.380%
14	16.028	2176	2183	2187	rBV	50114	98865	1.30%	0.198%
15	16.145	2196	2203	2208	rBV2	83333	152929	2.01%	0.306%
16	16.275	2217	2225	2243	rBV	3008583	4478598	58.96%	8.947%
17	16.486	2256	2261	2279	rVB	186421	351190	4.62%	0.702%
18	17.286	2392	2397	2401	rBV	168550	214269	2.82%	0.428%
19	17.339	2401	2406	2410	rVB2	60517	89209	1.17%	0.178%
20	17.545	2434	2441	2447	rBV	1732302	2534396	33.36%	5.063%
21	18.022	2518	2522	2527	rVB	175908	201179	2.65%	0.402%
22	18.186	2547	2550	2555	rVB	69177	86827	1.14%	0.173%
23	18.398	2582	2586	2592	rBV	251155	336492	4.43%	0.672%
24	18.686	2631	2635	2639	rBV	148314	170270	2.24%	0.340%
25	19.286	2733	2737	2739	rBV2	246757	301022	3.96%	0.601%
26	19.316	2739	2742	2754	rVB2	194215	281090	3.70%	0.562%
27	19.622	2791	2794	2801	rBV	95406	126144	1.66%	0.252%
28	19.845	2829	2832	2836	rBV	102490	109246	1.44%	0.218%
29	19.886	2836	2839	2845	rVB3	56388	78629	1.04%	0.157%
30	20.074	2866	2871	2881	rVB	6257498	7595988	100.00%	15.175%
31	20.363	2917	2920	2924	rBV2	109874	123974	1.63%	0.248%
32	20.845	2999	3002	3006	rBV2	106409	117903	1.55%	0.236%
33	21.298	3076	3079	3084	rBV	212879	263364	3.47%	0.526%
34	21.627	3129	3135	3140	rBV	1880668	2698876	35.53%	5.392%
35	24.209	3568	3574	3586	rVB2	1298572	2901452	38.20%	5.796%

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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_P\Methods\8270E-BP012623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

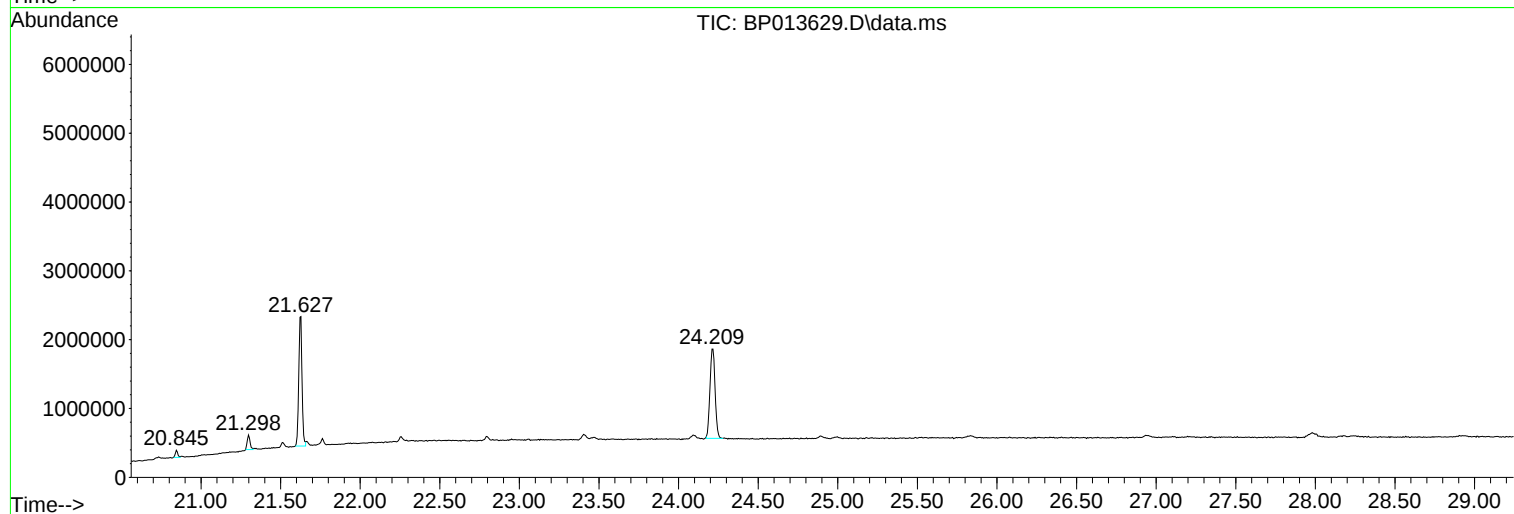
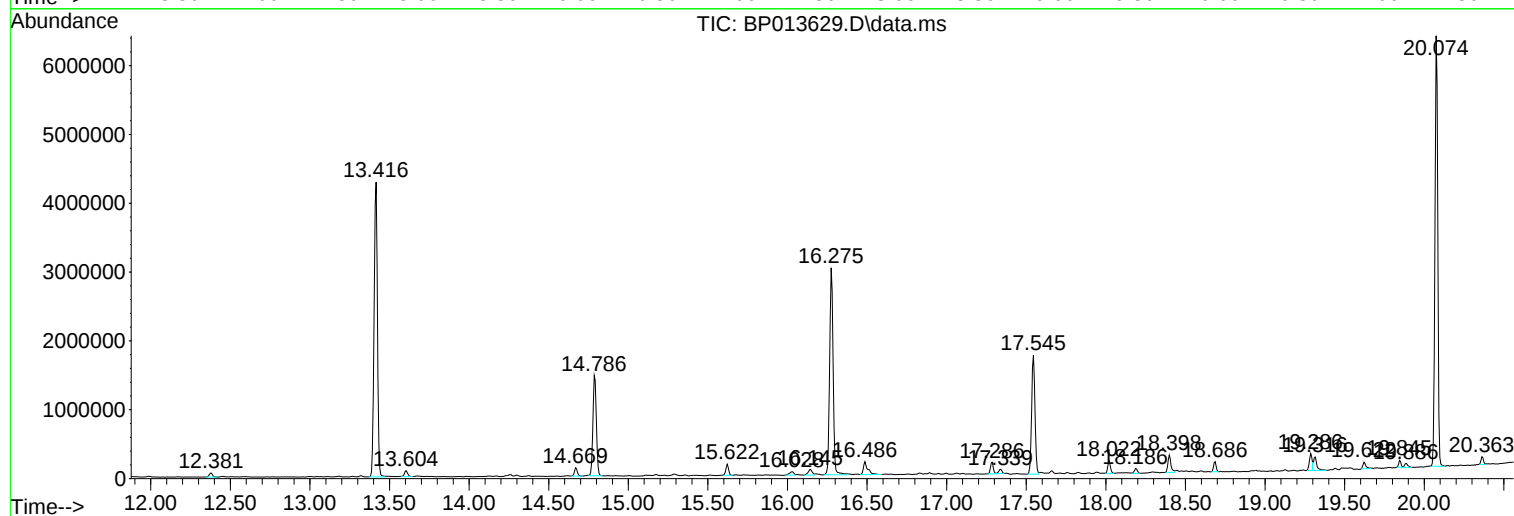
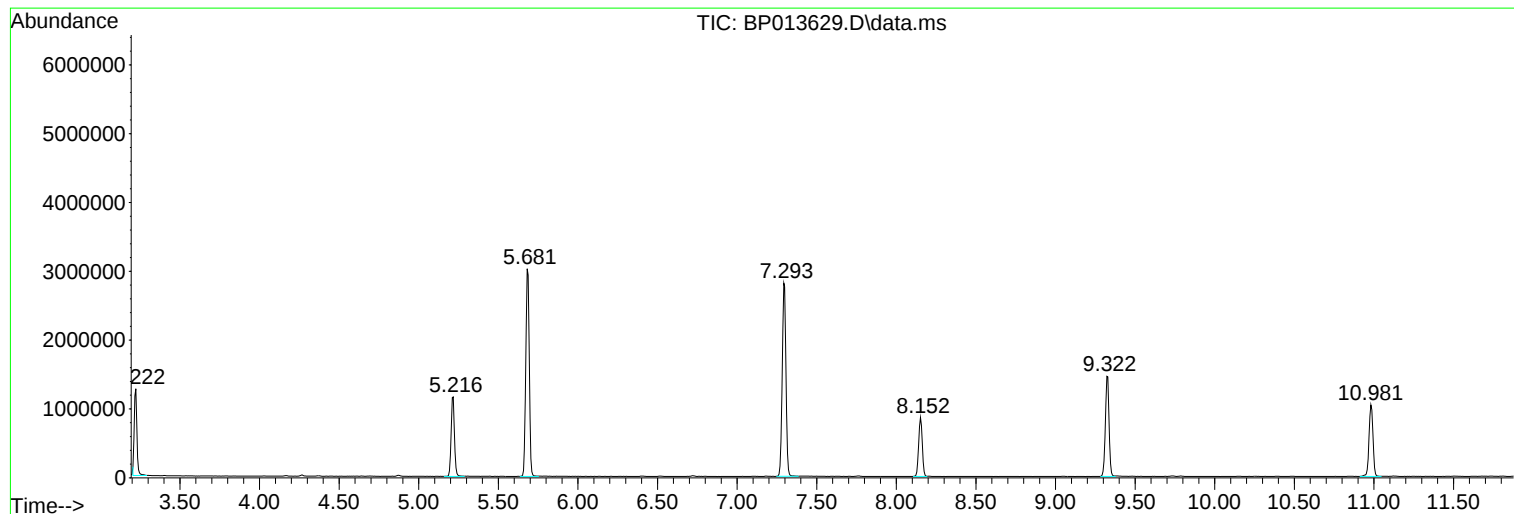
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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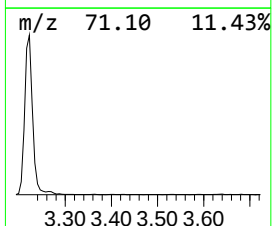
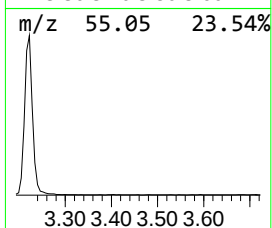
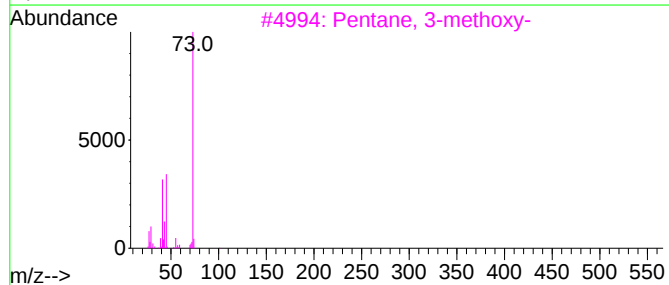
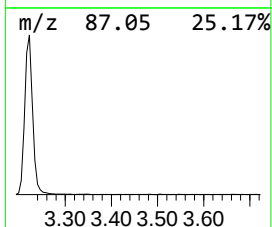
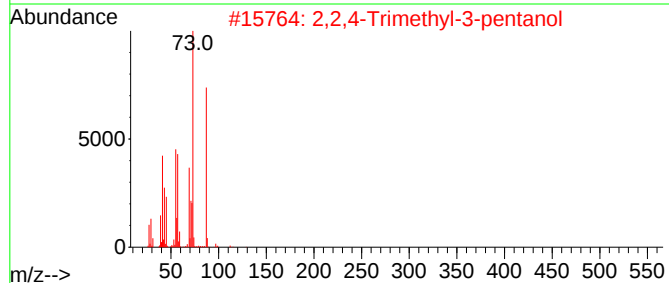
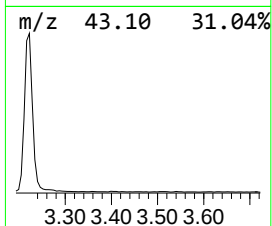
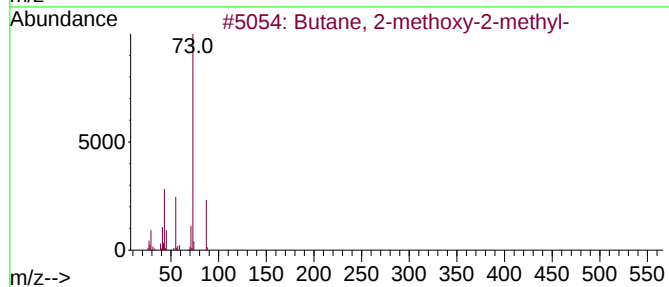
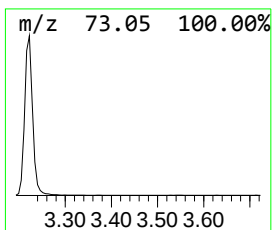
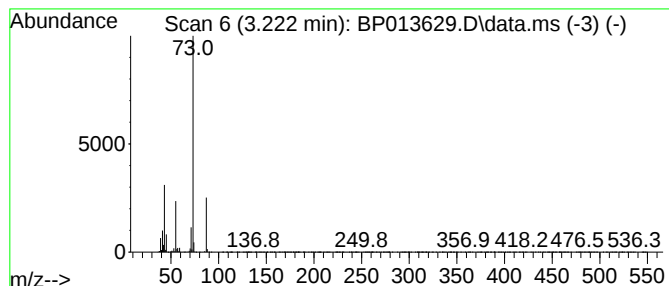
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	21.67 ng	1459150	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	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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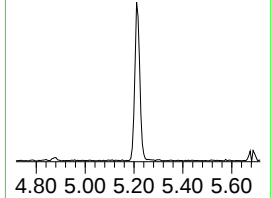
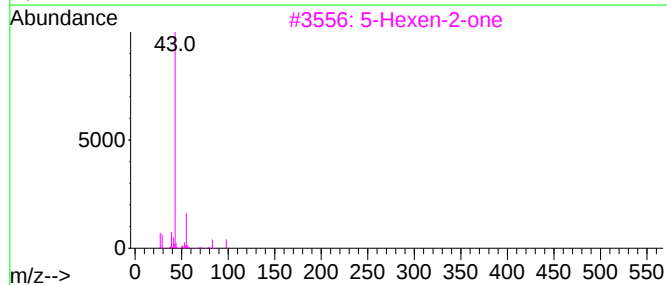
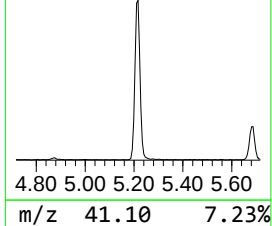
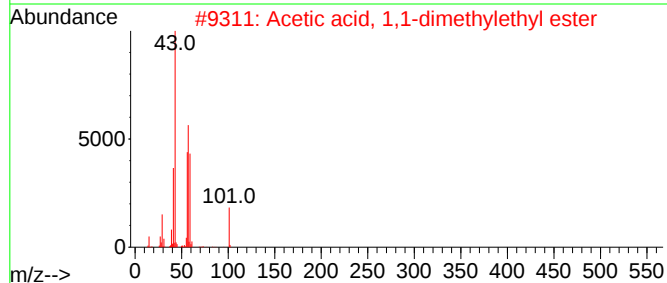
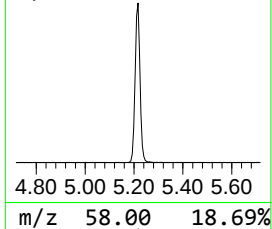
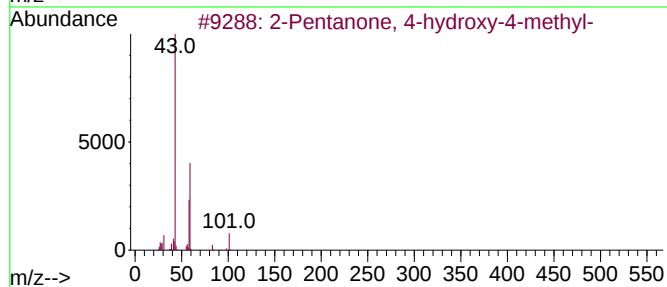
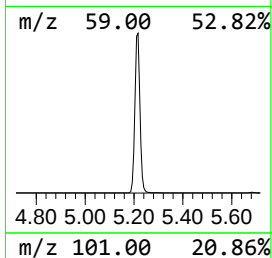
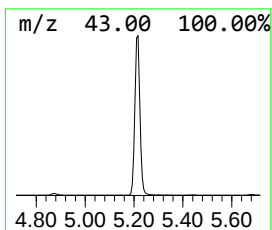
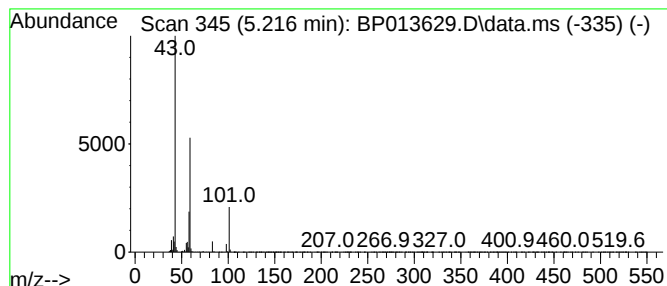
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	25.12 ng	1691750	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	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Acetone	58	C3H6O	000067-64-1	9		



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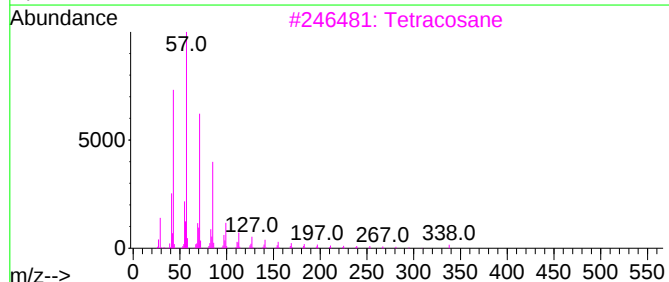
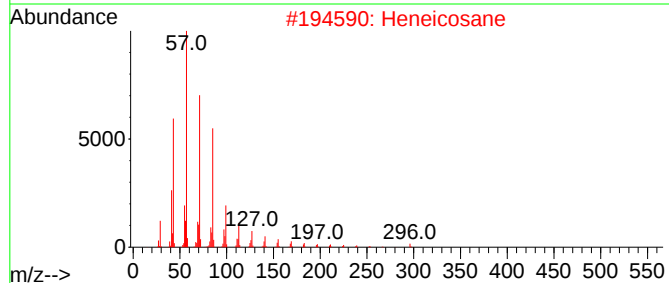
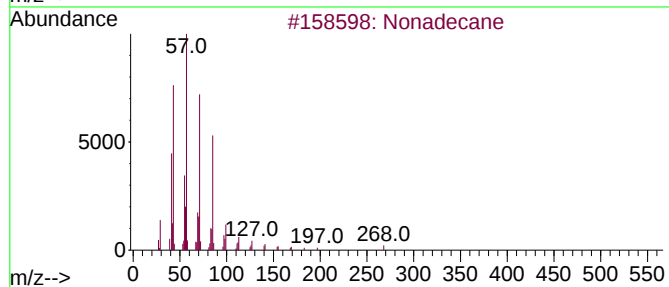
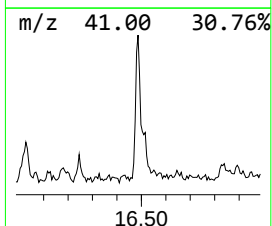
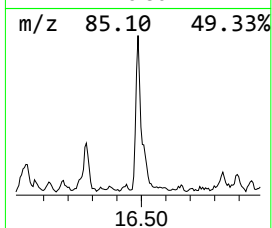
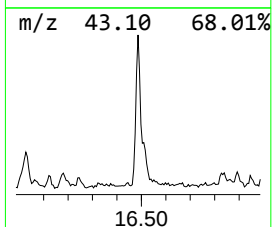
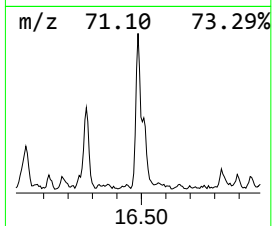
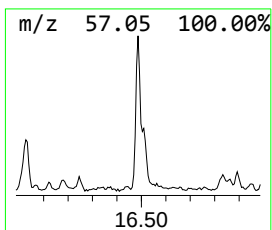
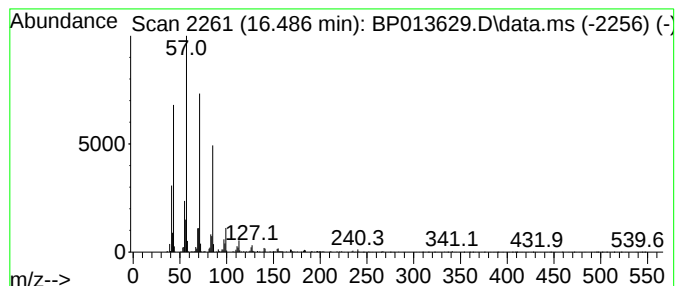
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.486	2.77 ng	351190	Phenanthrene-d10	17.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Heneicosane	296	C21H44	000629-94-7	87
3			Tetracosane	338	C24H50	000646-31-1	86
4			Dodecane, 4-methyl-	184	C13H28	006117-97-1	86
5			Tetradecane	198	C14H30	000629-59-4	86



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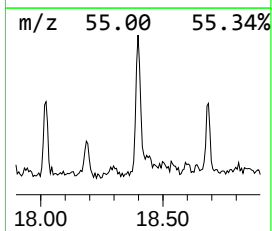
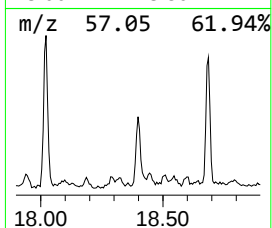
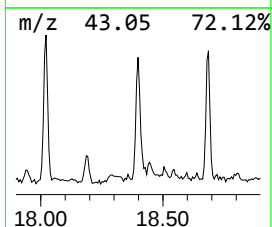
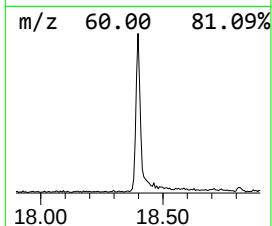
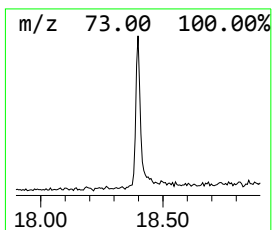
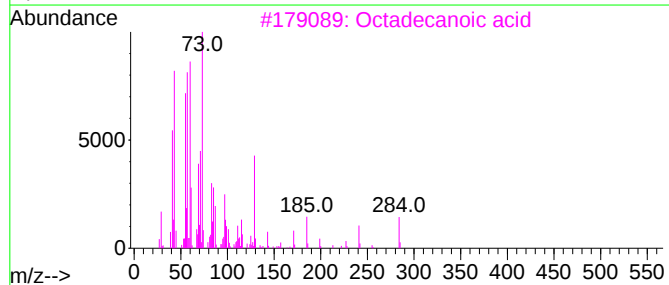
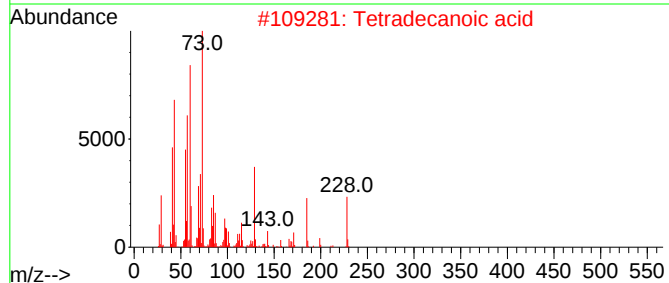
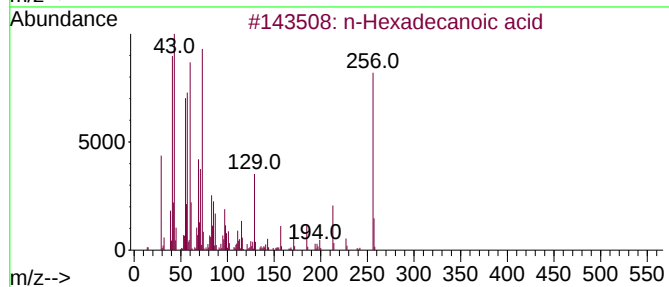
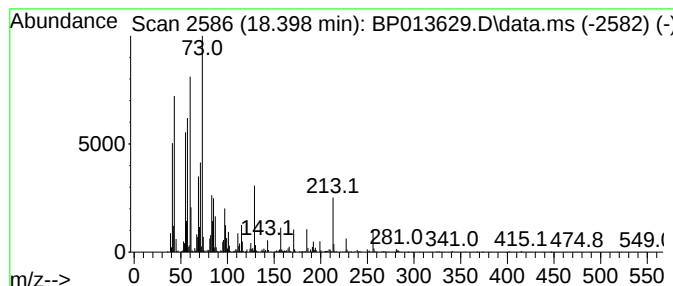
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.398	2.66 ng	336492	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	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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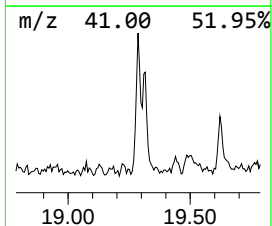
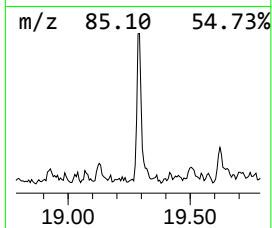
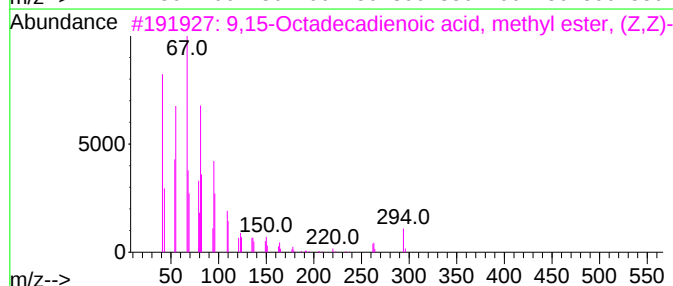
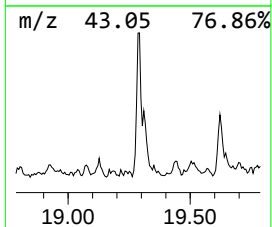
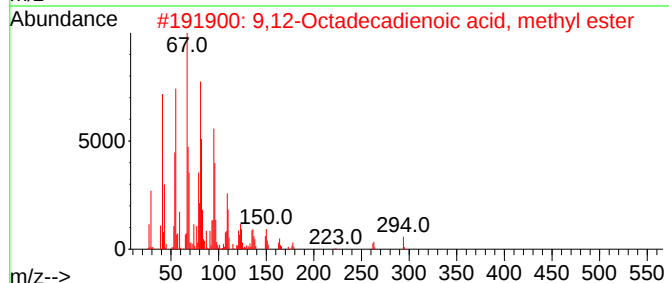
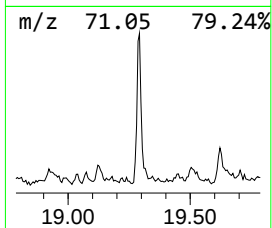
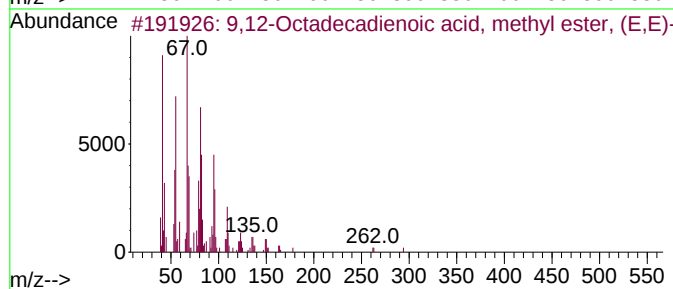
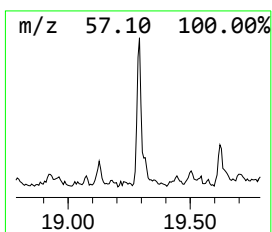
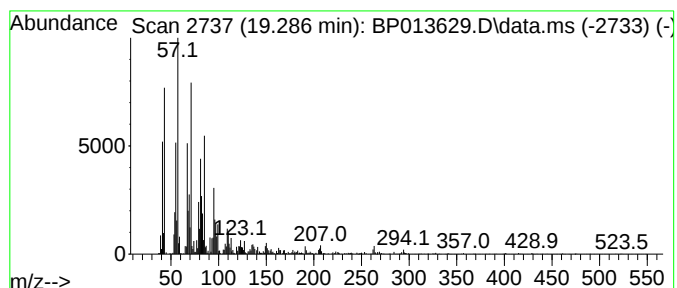
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.286	2.38 ng	301022	Phenanthrene-d10	17.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	94
2			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	93
3			9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	81
4			9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	81
5			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012723\
Data File : BP013629.D
Acq On : 27 Jan 2023 21:41
Operator : CG/JU
Sample : 01214-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

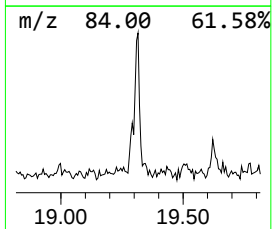
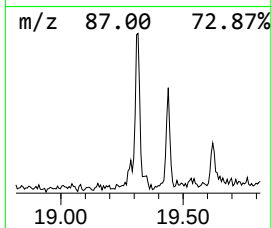
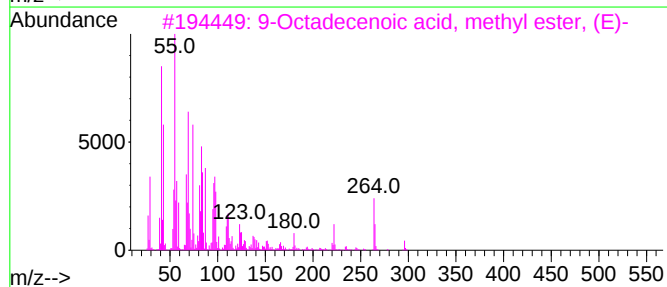
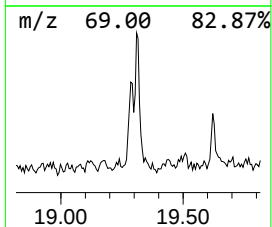
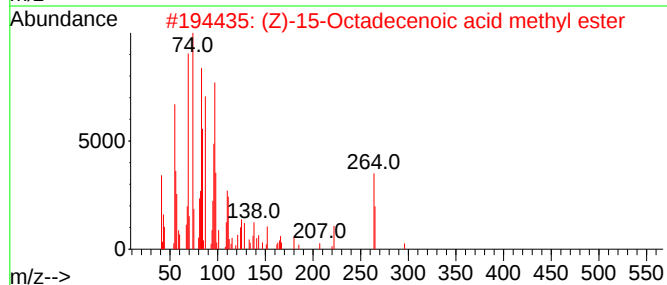
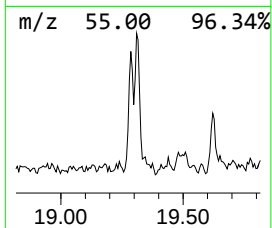
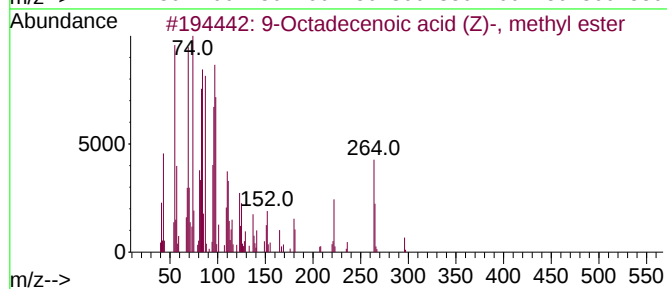
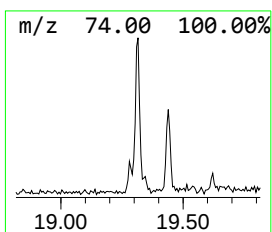
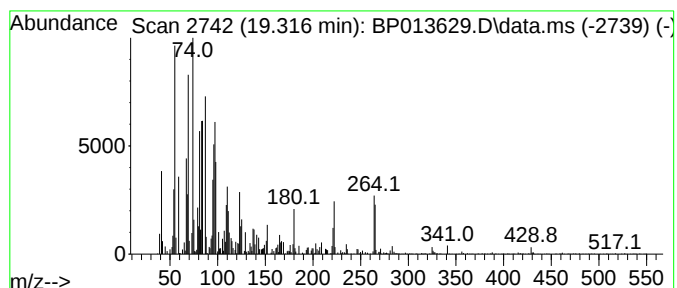
Instrument :
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ClientSampleId :
TJRC-011823-B3-20-30

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 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.316	2.22 ng	281090	Phenanthrene-d10	17.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
2	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	87
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	76
4	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	76
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012723\
Data File : BP013629.D
Acq On : 27 Jan 2023 21:41
Operator : CG/JU
Sample : 01214-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TJRC-011823-B3-20-30

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.222	21.7	ng	1459150	1	8.152	1346680	20.0
2-Pentanone, 4-...	5.216	25.1	ng	1691750	1	8.152	1346680	20.0
Nonadecane	16.486	2.8	ng	351190	4	17.545	2534400	20.0
n-Hexadecanoic ...	18.398	2.7	ng	336492	4	17.545	2534400	20.0
9,12-Octadecadi...	19.286	2.4	ng	301022	4	17.545	2534400	20.0
9-Octadecenoic ...	19.316	2.2	ng	281090	4	17.545	2534400	20.0