

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
 Data File : BP006518.D
 Acq On : 05 Aug 2021 22:04
 Operator : CG/JU
 Sample : M3279-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20210569-COM-42

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-BP080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.905	304	309	322	rVB	1624392	2218817	25.19%	3.716%
2	5.358	380	386	397	rVB	4225455	5811239	65.96%	9.734%
3	5.969	485	490	498	rVB	329841	467950	5.31%	0.784%
4	6.934	647	654	667	rVB	3985108	6124108	69.51%	10.258%
5	7.752	787	793	801	rBV	902755	1431158	16.25%	2.397%
6	8.911	982	990	1000	rBV	2362691	3845744	43.65%	6.442%
7	10.328	1224	1231	1243	rBV	362894	608933	6.91%	1.020%
8	10.540	1259	1267	1274	rBV	1220716	2019475	22.92%	3.383%
9	11.816	1476	1484	1491	rVB	51944	114716	1.30%	0.192%
10	13.010	1678	1687	1700	rBV	4782705	6867118	77.95%	11.502%
11	13.816	1816	1824	1829	rBV2	58114	100025	1.14%	0.168%
12	14.381	1912	1920	1928	rBV	1641898	2503709	28.42%	4.194%
13	15.875	2161	2174	2196	rBV	4034149	5823115	66.10%	9.754%
14	17.134	2381	2388	2396	rBV	1962201	2854068	32.40%	4.781%
15	18.039	2537	2542	2551	rBV	275813	398499	4.52%	0.667%
16	19.281	2749	2753	2760	rBV	152466	205729	2.34%	0.345%
17	19.539	2793	2797	2801	rVB2	129729	154971	1.76%	0.260%
18	19.710	2820	2826	2831	rBV	7219138	8809801	100.00%	14.756%
19	20.022	2876	2879	2883	rVB	154379	157382	1.79%	0.264%
20	20.504	2957	2961	2965	rBV2	271133	332209	3.77%	0.556%
21	20.963	3035	3039	3046	rBV	551054	652676	7.41%	1.093%
22	21.233	3080	3085	3091	rBV	2453870	3079169	34.95%	5.158%
23	21.398	3109	3113	3117	rVB	374357	408295	4.63%	0.684%
24	21.845	3186	3189	3197	rVB	343149	444313	5.04%	0.744%
25	22.333	3268	3272	3279	rVB	279831	402957	4.57%	0.675%
26	22.463	3291	3294	3299	rVB	257236	345421	3.92%	0.579%
27	22.869	3360	3363	3369	rVB	223063	309795	3.52%	0.519%
28	23.557	3473	3480	3491	rVB2	1585046	3210560	36.44%	5.378%

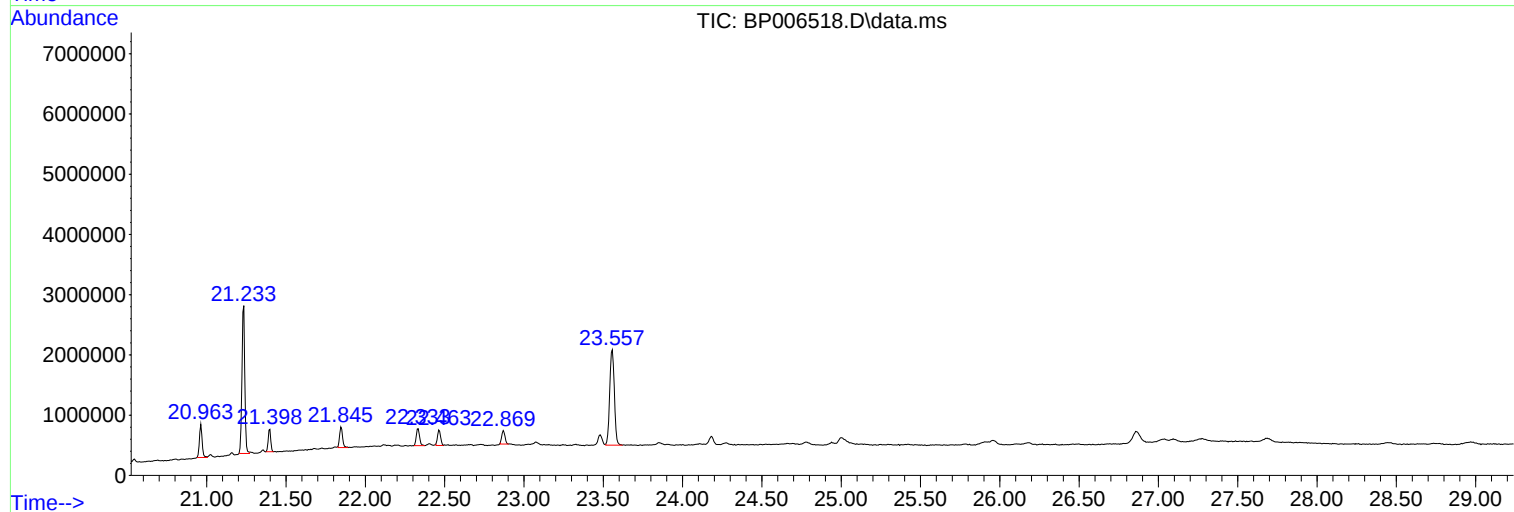
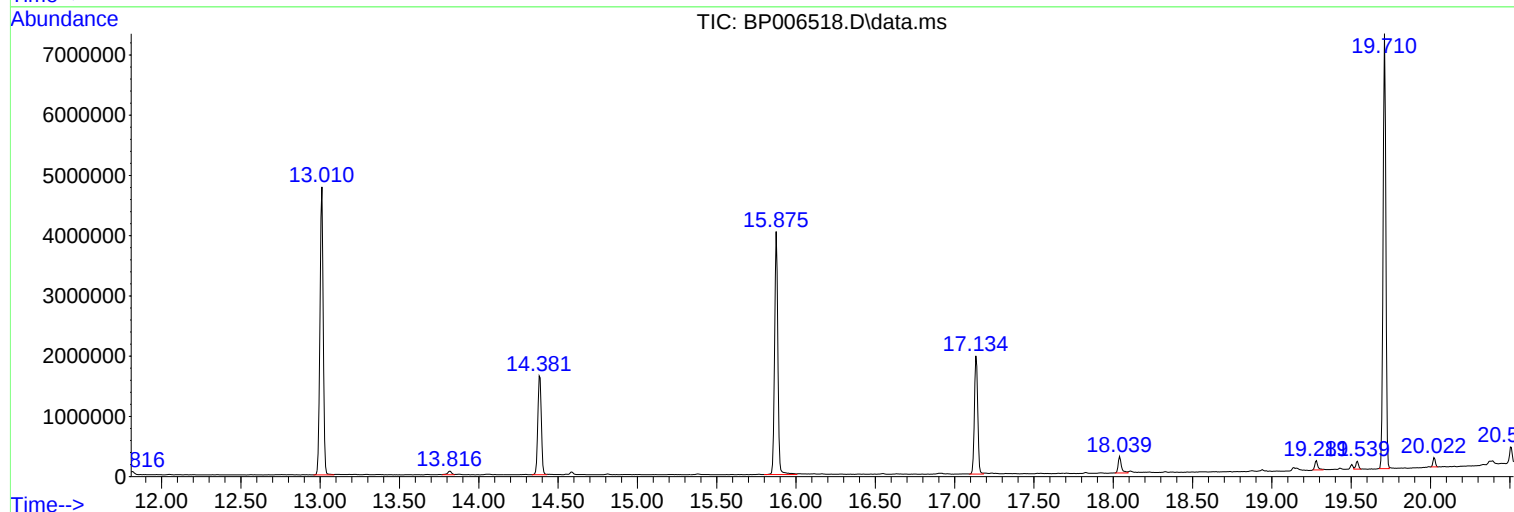
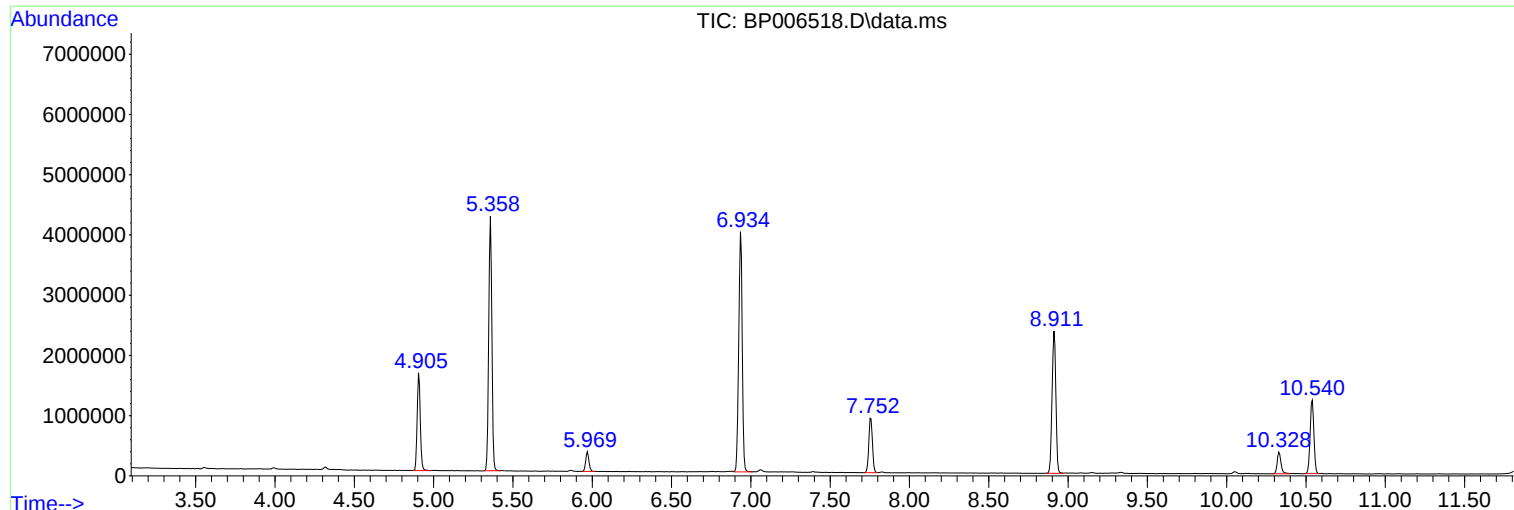
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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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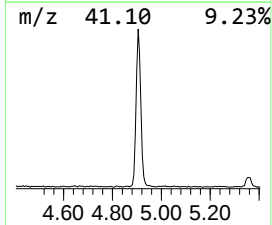
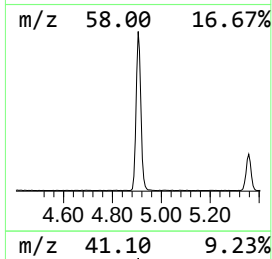
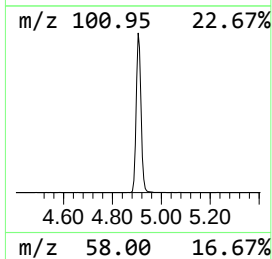
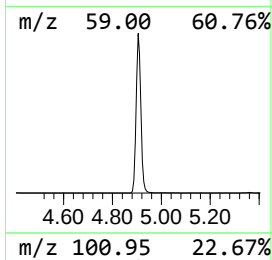
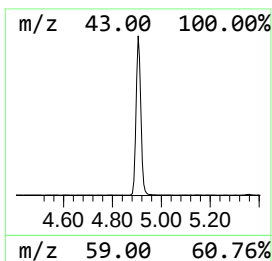
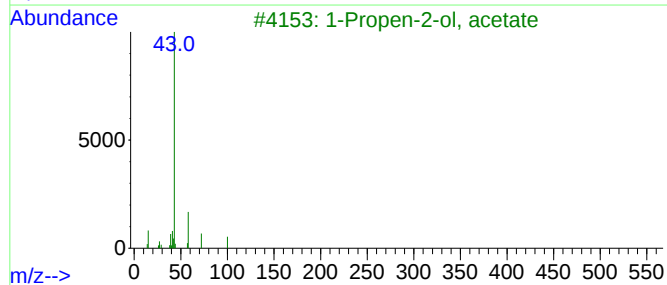
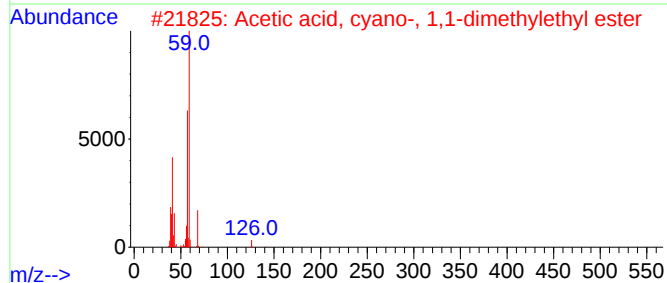
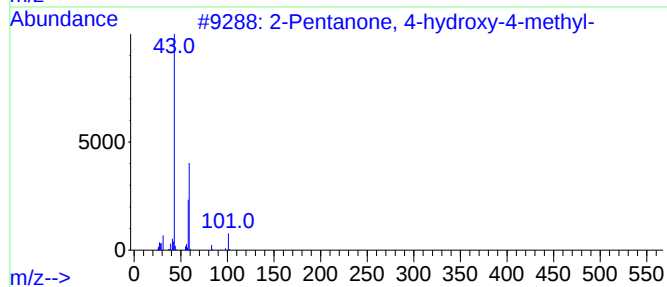
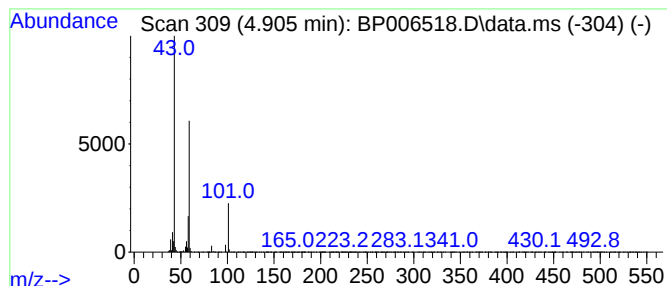
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	31.01 ng	2218820	1,4-Dichlorobenzene-d4	7.758

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Acetone	58	C3H6O	000067-64-1	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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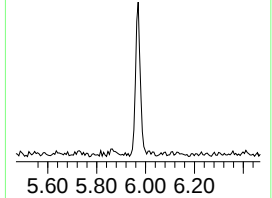
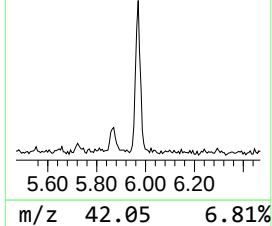
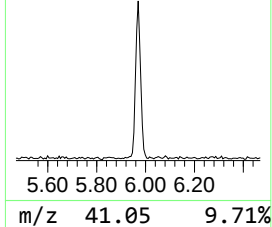
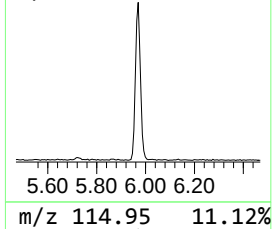
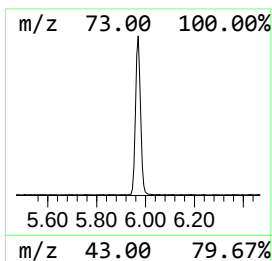
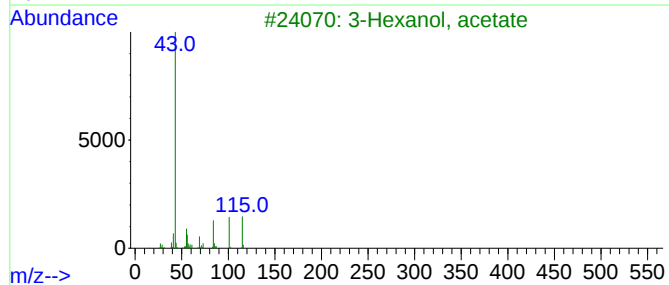
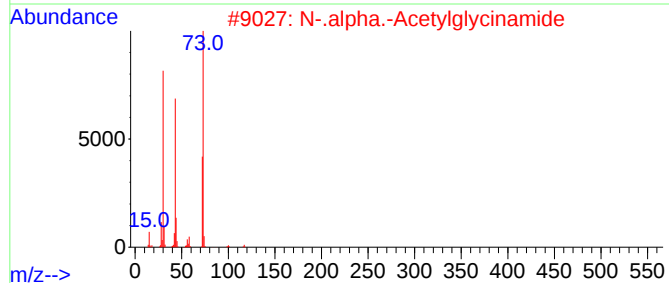
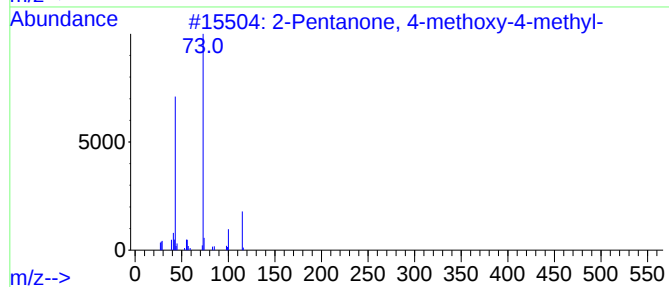
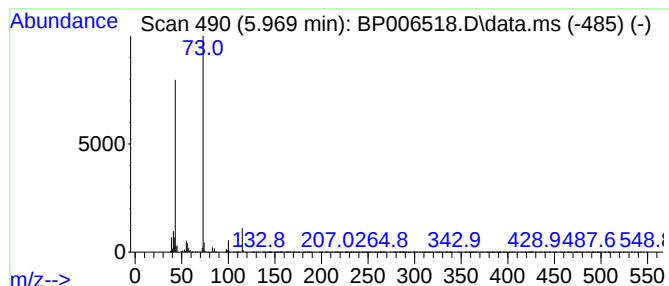
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	6.54 ng	467950	1,4-Dichlorobenzene-d4	7.758

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
3			3-Hexanol, acetate	144	C8H16O2	040780-64-1	25
4			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10



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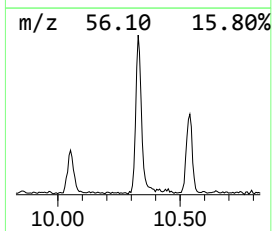
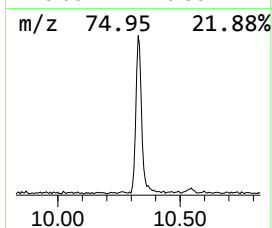
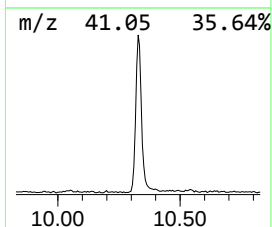
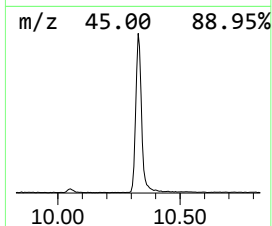
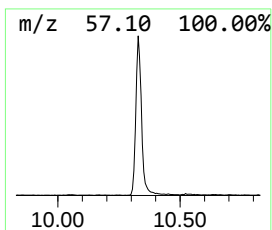
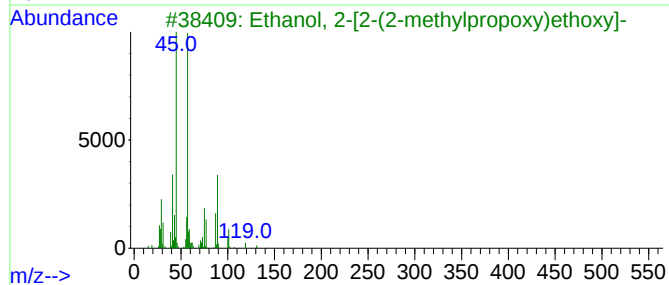
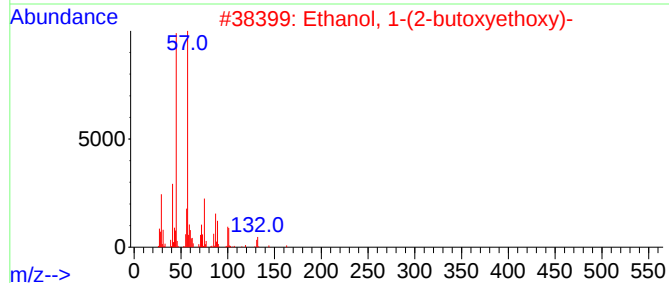
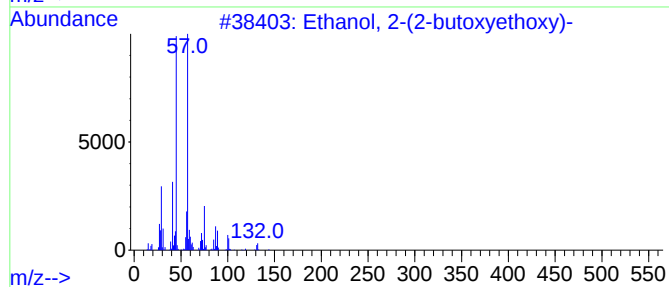
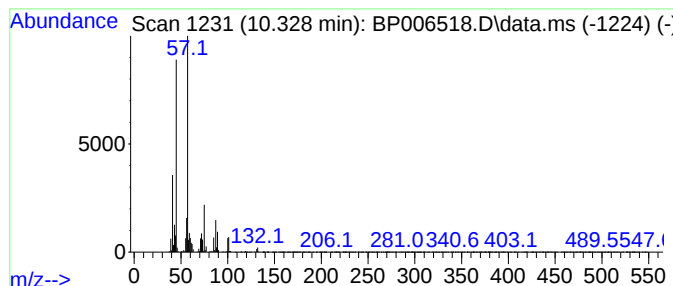
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	6.03 ng	608933	Naphthalene-d8	10.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Diisopropyl ether	102	C6H14O	000108-20-3	46



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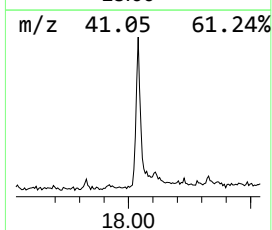
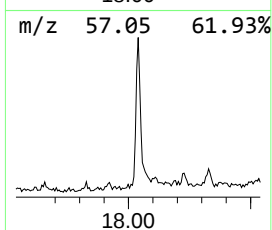
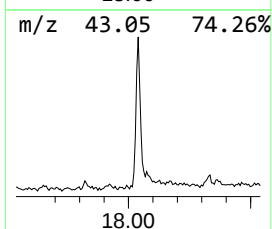
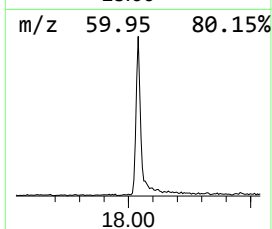
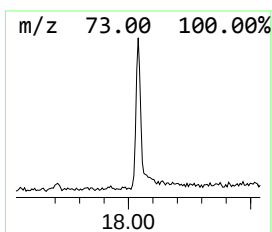
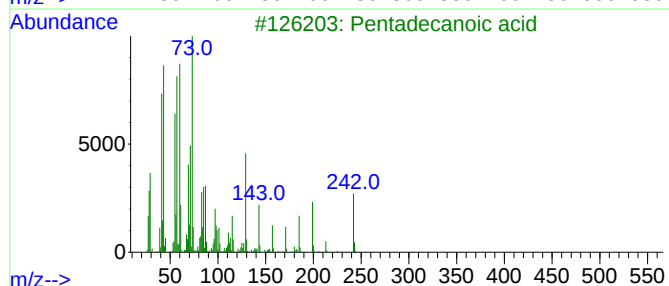
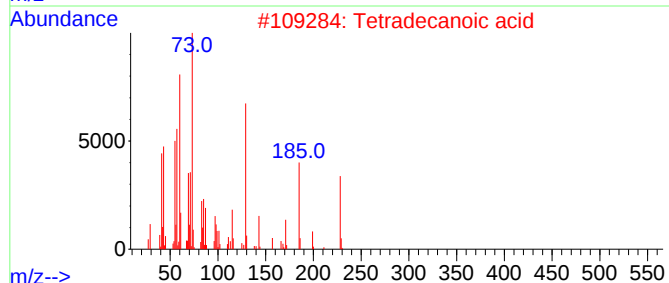
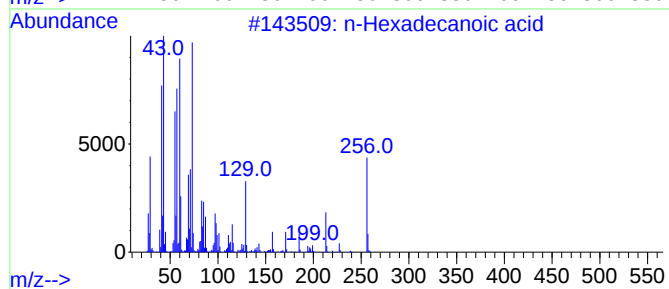
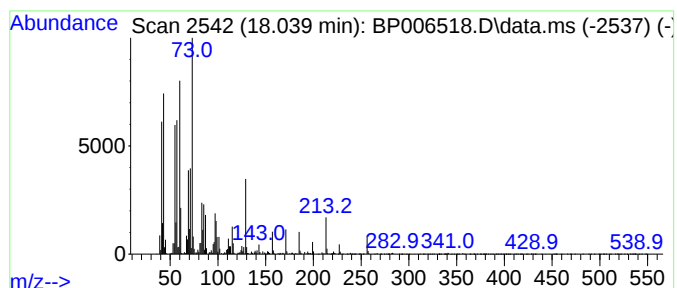
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.040	2.79 ng	398499	Phenanthrene-d10	17.134

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	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Octadecanoic acid	284	C18H36O2	000057-11-4	80
5		Tridecanoic acid	214	C13H26O2	000638-53-9	70



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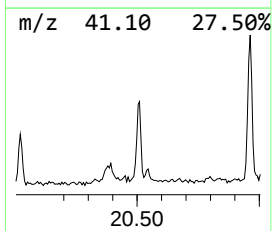
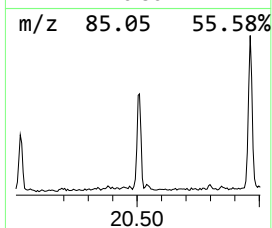
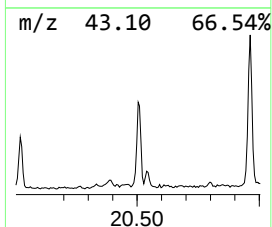
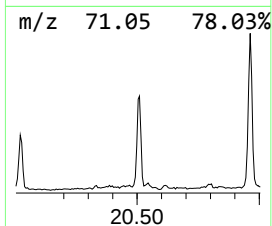
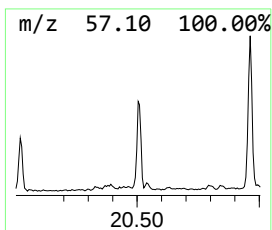
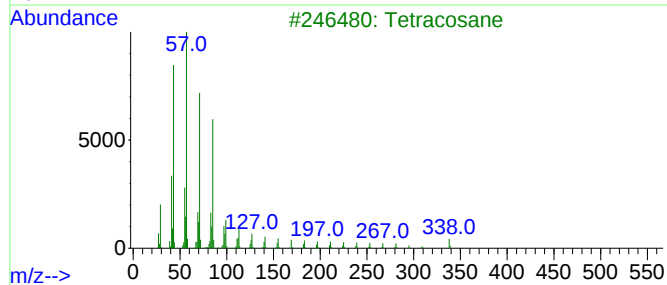
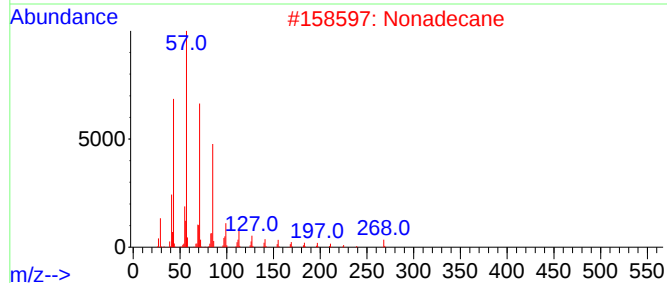
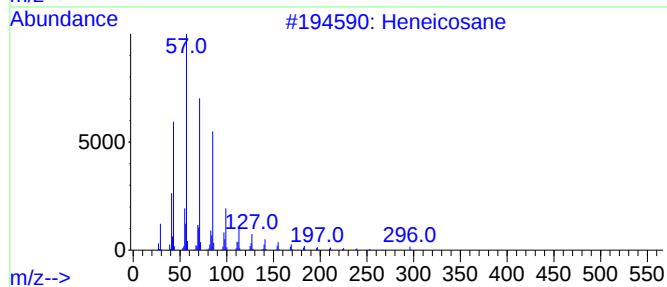
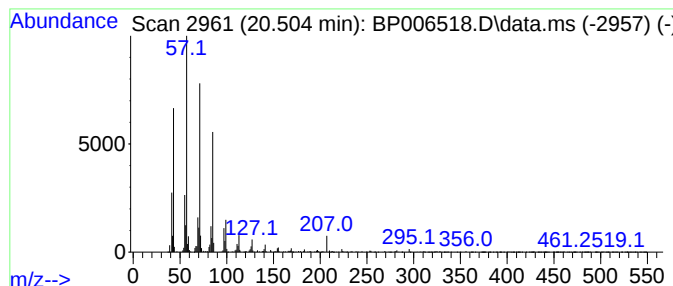
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Peak Number 5 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.504	2.16 ng	332209	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Nonadecane	268	C19H40	000629-92-5	86
3			Tetracosane	338	C24H50	000646-31-1	86
4			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	83
5			2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1010280-67-0	80



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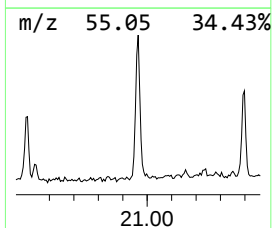
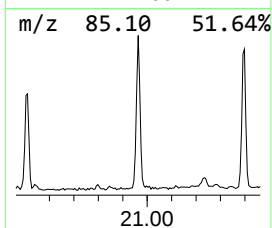
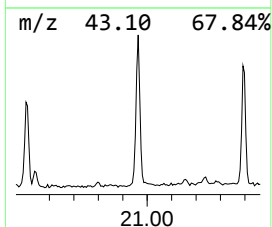
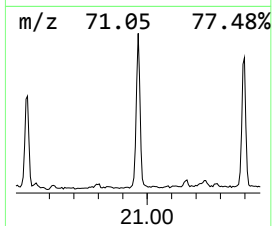
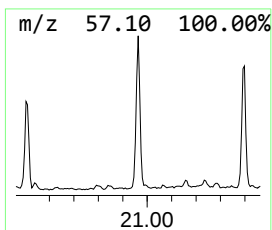
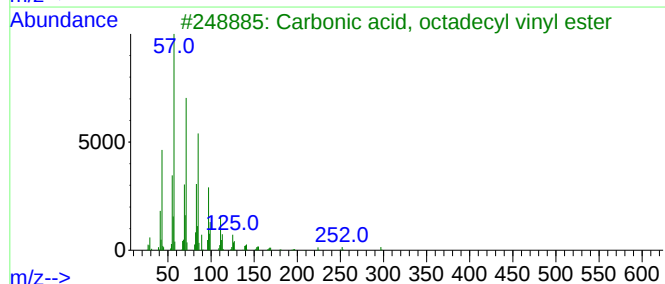
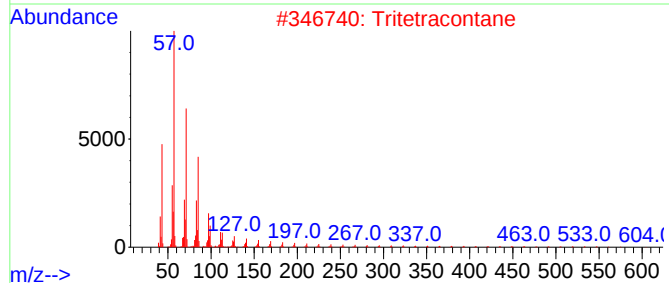
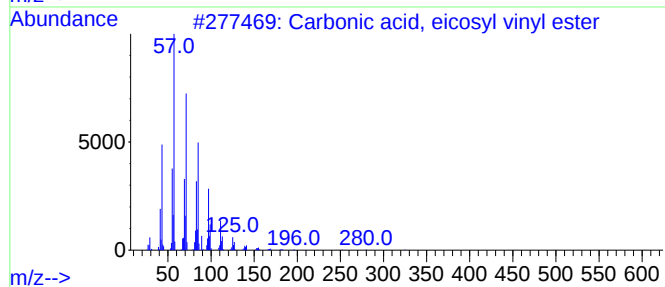
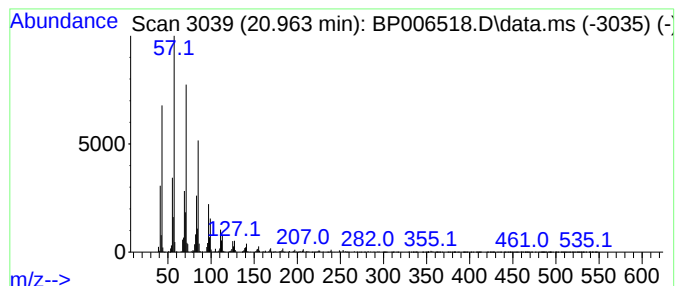
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, eicosyl vinyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	4.24 ng	652676	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
2			Tritetracontane	605	C43H88	007098-21-7	91
3			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	91
4			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	91
5			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006518.D
Acq On : 05 Aug 2021 22:04
Operator : CG/JU
Sample : M3279-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210569-COM-42

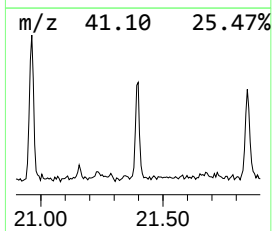
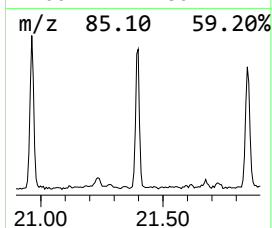
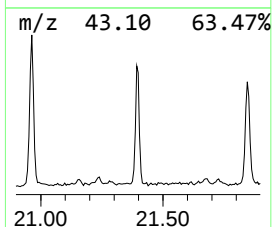
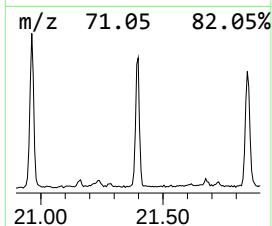
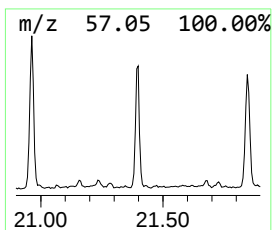
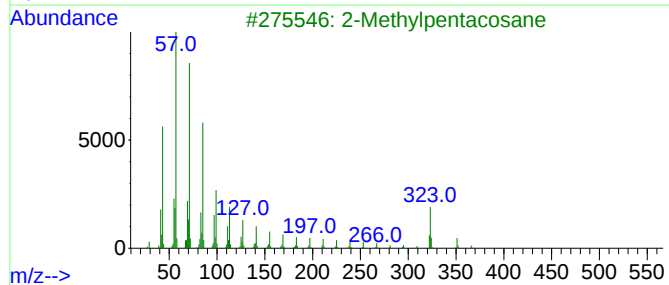
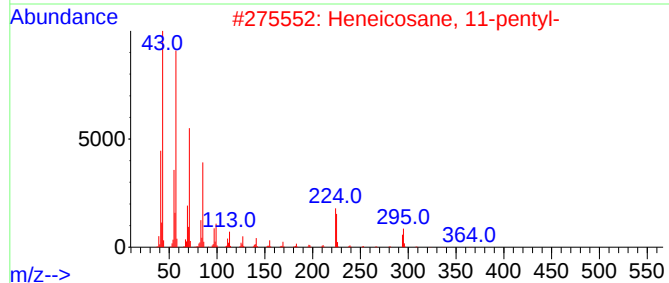
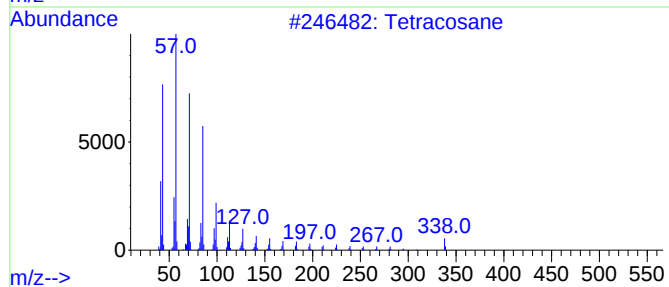
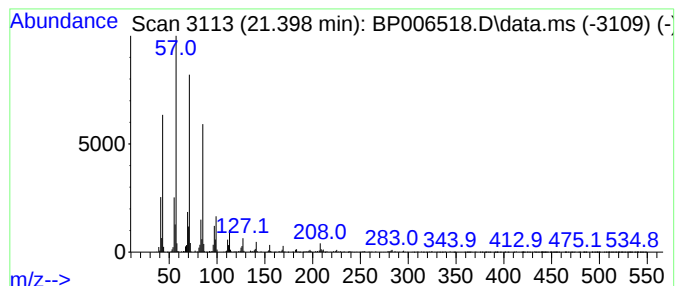
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.398	2.65 ng	408295	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	96
2			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	91
3			2-Methylpentacosane	366	C26H54	000629-87-8	91
4			Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006518.D
Acq On : 05 Aug 2021 22:04
Operator : CG/JU
Sample : M3279-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210569-COM-42

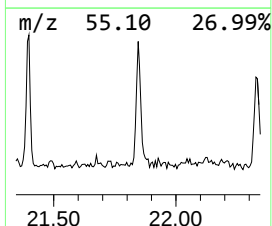
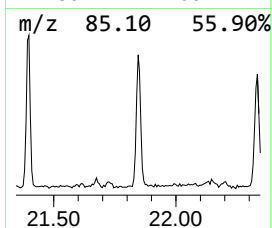
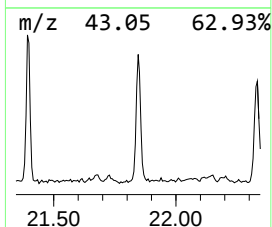
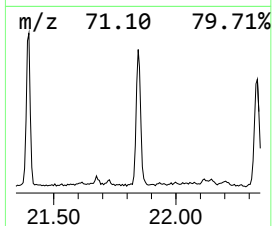
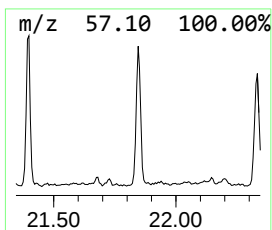
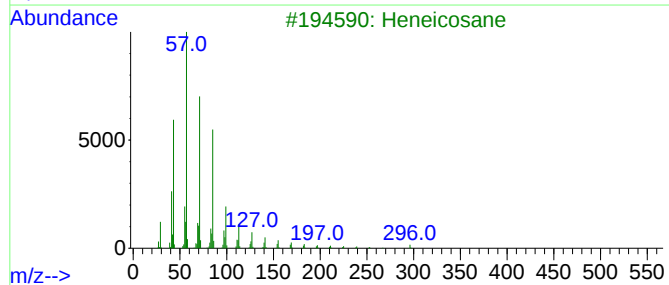
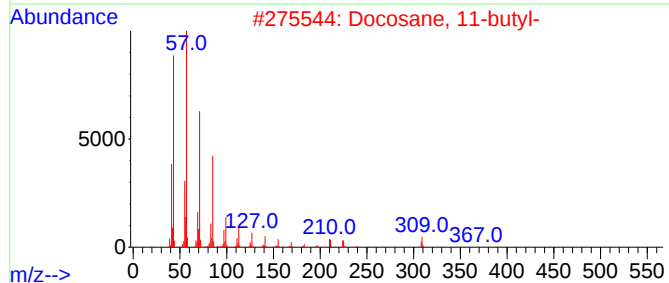
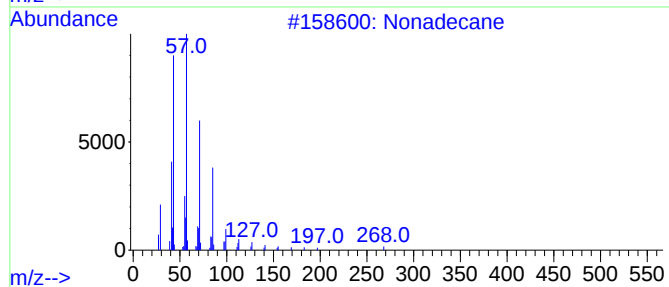
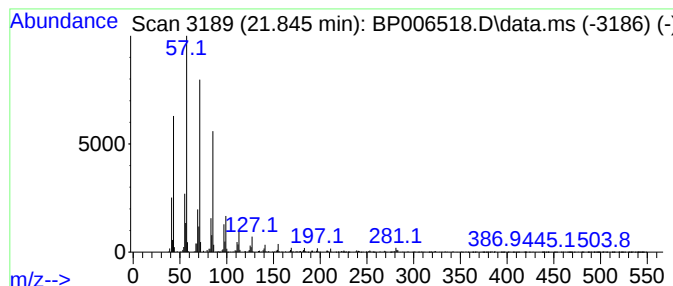
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.845	2.89 ng	444313	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	96
2			Docosane, 11-butyl-	366	C26H54	013475-76-8	94
3			Heneicosane	296	C21H44	000629-94-7	91
4			Hexacosane	366	C26H54	000630-01-3	90
5			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006518.D
Acq On : 05 Aug 2021 22:04
Operator : CG/JU
Sample : M3279-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210569-COM-42

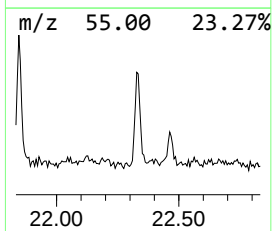
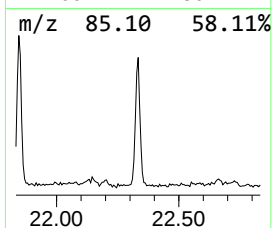
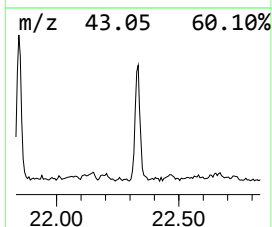
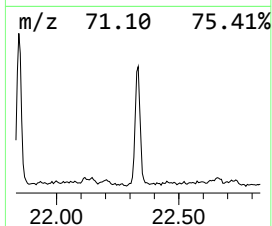
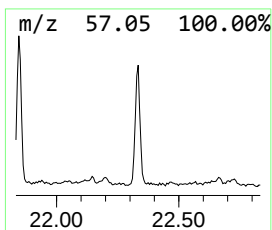
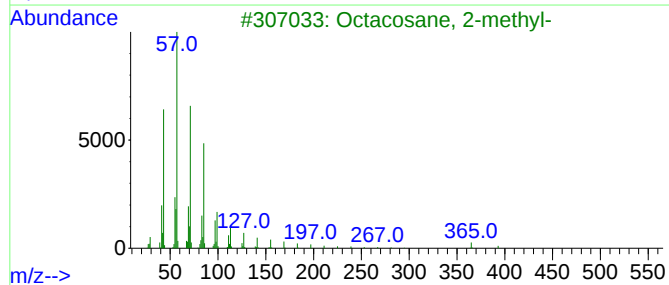
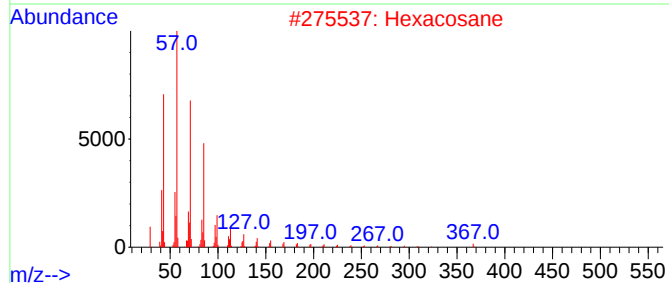
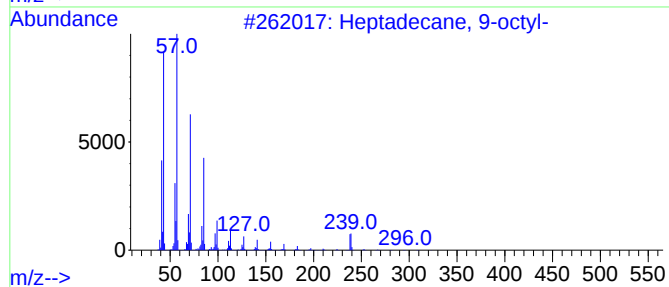
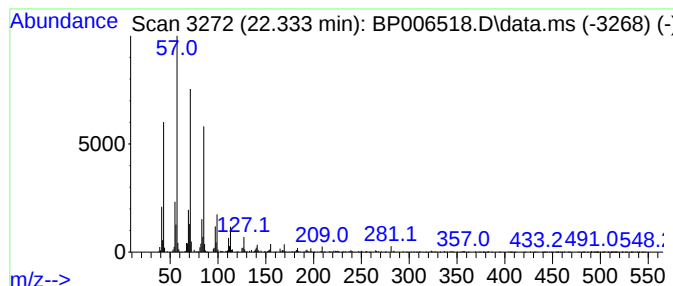
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.333	2.62 ng	402957	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006518.D
Acq On : 05 Aug 2021 22:04
Operator : CG/JU
Sample : M3279-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20210569-COM-42

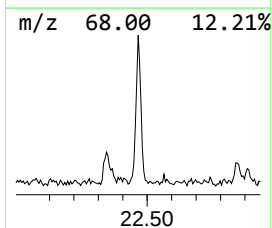
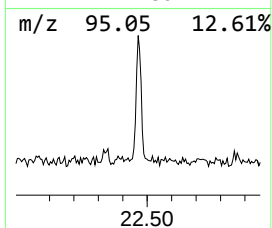
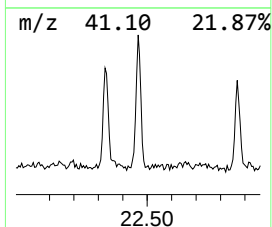
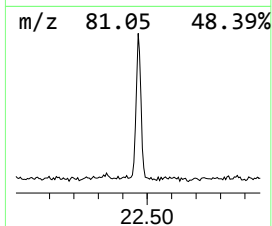
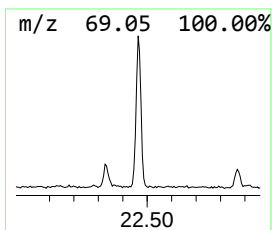
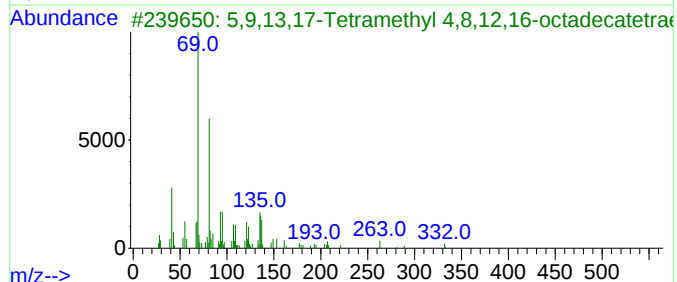
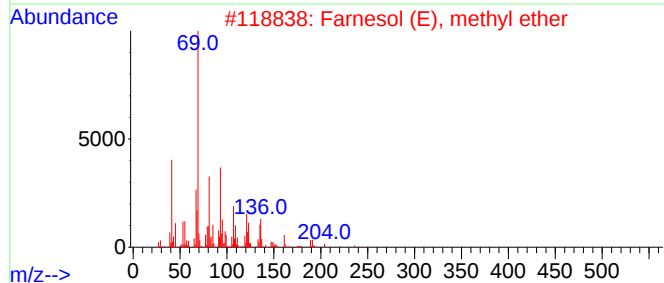
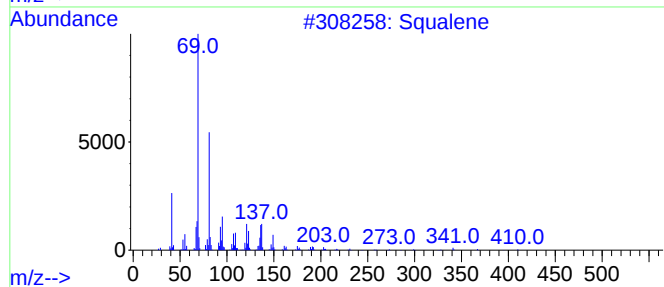
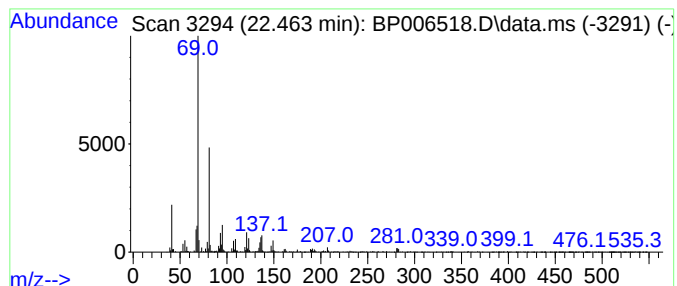
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.463	2.15 ng	345421	Perylene-d12	23.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	78
3			5,9,13,17-Tetramethyl 4,8,12,16-...	332	C22H36O2	1000432-37-9	72
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5			2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	003675-00-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
Data File : BP006518.D
Acq On : 05 Aug 2021 22:04
Operator : CG/JU
Sample : M3279-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20210569-COM-42

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.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
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2-Pentanone, 4-...	5.969	6.5	ng	467950	1	7.758	1431160	20.0
Ethanol, 2-(2-b...	10.328	6.0	ng	608933	2	10.540	2019480	20.0
n-Hexadecanoic ...	18.040	2.8	ng	398499	4	17.134	2854070	20.0
Heneicosane	20.504	2.2	ng	332209	5	21.233	3079170	20.0
Carbonic acid, ...	20.963	4.2	ng	652676	5	21.233	3079170	20.0
Tetracosane	21.398	2.6	ng	408295	5	21.233	3079170	20.0
Nonadecane	21.845	2.9	ng	444313	5	21.233	3079170	20.0
Heptadecane, 9-...	22.333	2.6	ng	402957	5	21.233	3079170	20.0
Squalene	22.463	2.1	ng	345421	6	23.557	3210560	20.0