

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060624\
 Data File : BP020552.D
 Acq On : 06 Jun 2024 22:44
 Operator : MA/JU
 Sample : P2715-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 WCS-TPC

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-BP052924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP020552.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	19	rVB	1690139	2178361	16.72%	2.736%
2	3.552	92	96	110	rBV	515497	703761	5.40%	0.884%
3	4.016	171	175	181	rVB	107993	150531	1.16%	0.189%
4	5.375	399	406	421	rBV	4349817	6322899	48.53%	7.942%
5	6.934	660	671	686	rBV	4123110	6740427	51.73%	8.467%
6	7.369	739	745	757	rBV	166564	271796	2.09%	0.341%
7	7.763	805	812	819	rBV	1001366	1539831	11.82%	1.934%
8	8.910	999	1007	1017	rBV	2575288	4368746	33.53%	5.488%
9	9.469	1092	1102	1113	rBV	145378	226640	1.74%	0.285%
10	10.539	1274	1284	1295	rBV	1318684	2223196	17.06%	2.793%
11	11.275	1399	1409	1421	rBV	467931	781945	6.00%	0.982%
12	13.004	1695	1703	1716	rBV	6489505	9889522	75.90%	12.423%
13	14.298	1918	1923	1928	rBV	142340	173121	1.33%	0.217%
14	14.392	1931	1939	1947	rVB	2014293	2970113	22.80%	3.731%
15	14.627	1977	1979	1992	rVB	3737783	4138461	31.76%	5.198%
16	15.269	2083	2088	2093	rVB	170548	234963	1.80%	0.295%
17	15.916	2190	2198	2206	rBV	5265801	8120618	62.33%	10.201%
18	16.151	2233	2238	2253	rVB	186404	421773	3.24%	0.530%
19	16.969	2373	2377	2382	rBV	1999999	278288	2.14%	0.350%
20	17.021	2383	2386	2395	rVB	75907	131514	1.01%	0.165%
21	17.198	2410	2416	2422	rBV	2439974	3389466	26.01%	4.258%
22	17.733	2503	2507	2513	rBV	178375	247440	1.90%	0.311%
23	18.145	2571	2577	2584	rBV	582227	924356	7.09%	1.161%
24	18.451	2625	2629	2634	rBV	164691	234368	1.80%	0.294%
25	18.892	2699	2704	2706	rBV6	82011	140471	1.08%	0.176%
26	19.115	2739	2742	2750	rVB2	165880	303813	2.33%	0.382%
27	19.357	2777	2783	2784	rBV5	70262	132731	1.02%	0.167%
28	19.474	2798	2803	2810	rVB2	238777	440205	3.38%	0.553%
29	19.727	2843	2846	2850	rBV	151466	173450	1.33%	0.218%
30	19.933	2874	2881	2886	rBV	8383704	13029258	100.00%	16.367%
31	20.410	2959	2962	2963	rBV2	134578	151546	1.16%	0.190%
32	21.339	3116	3120	3128	rVB2	560790	969511	7.44%	1.218%
33	21.657	3169	3174	3181	rVB	2086120	3327580	25.54%	4.180%
34	22.580	3327	3331	3337	rBV3	273919	552393	4.24%	0.694%
35	25.021	3739	3746	3757	rVB	1373897	3726043	28.60%	4.680%

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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-BP052924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

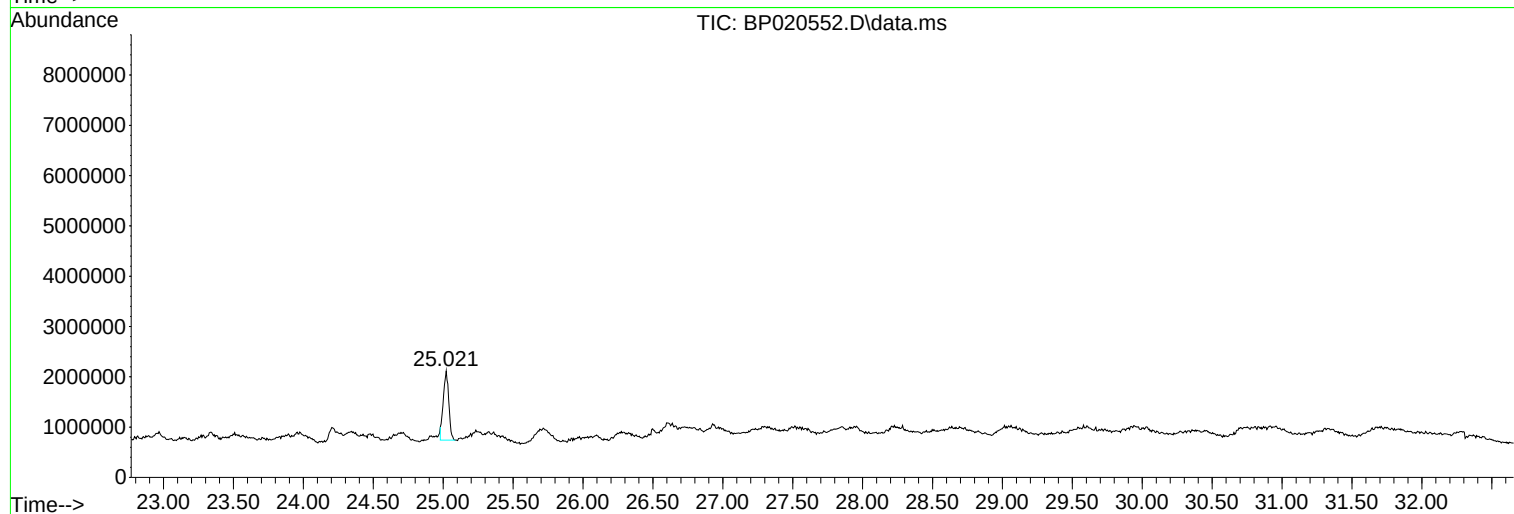
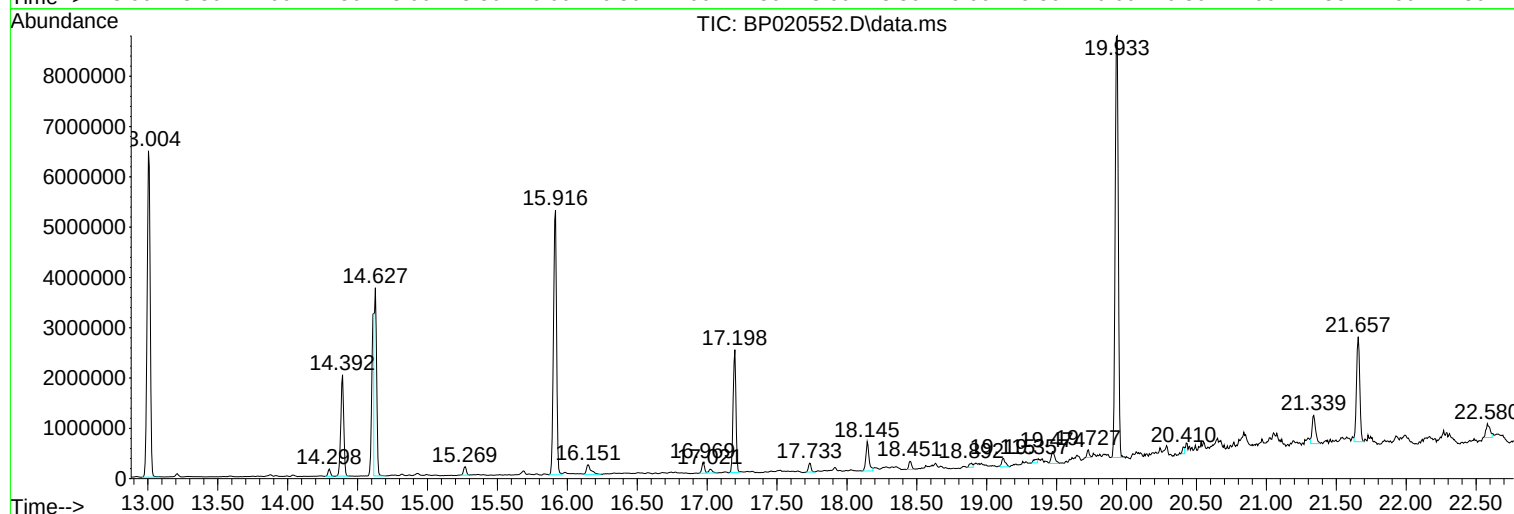
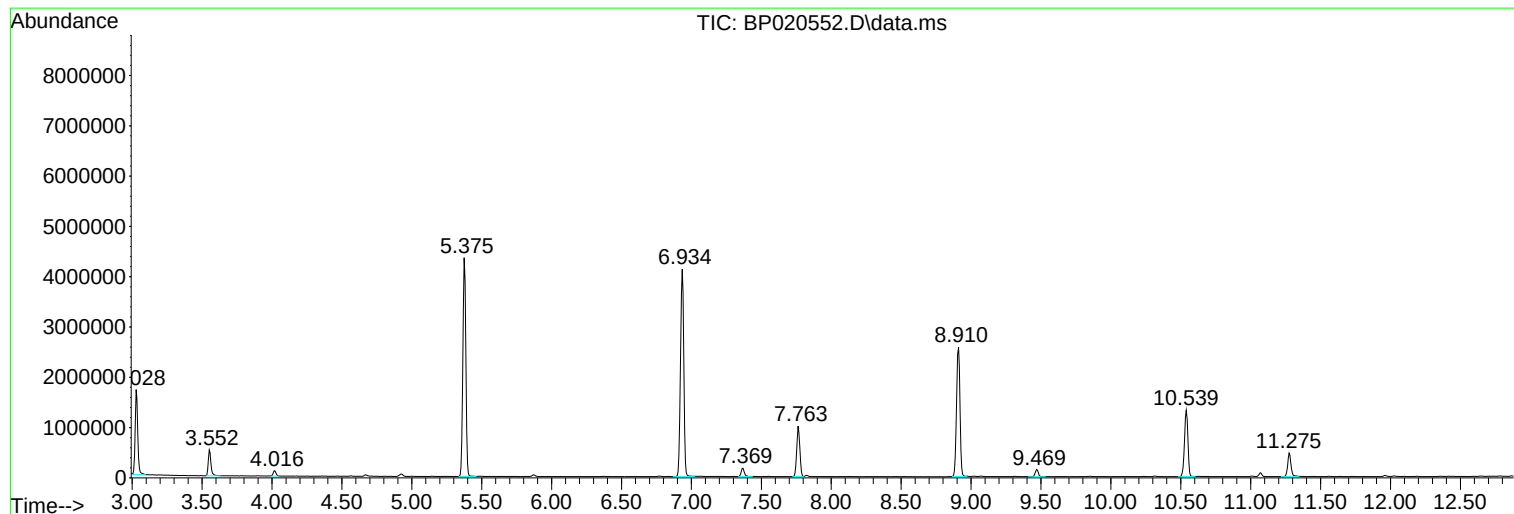
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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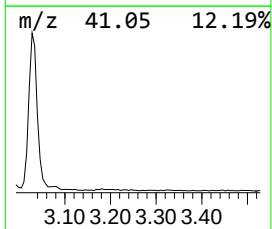
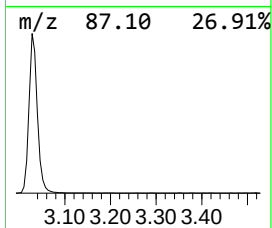
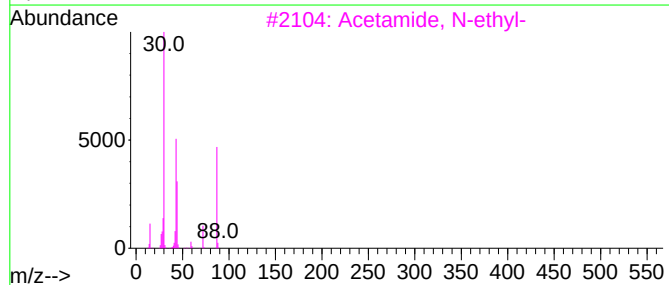
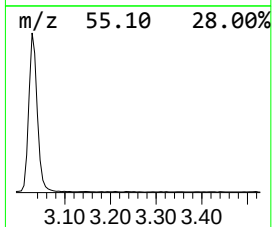
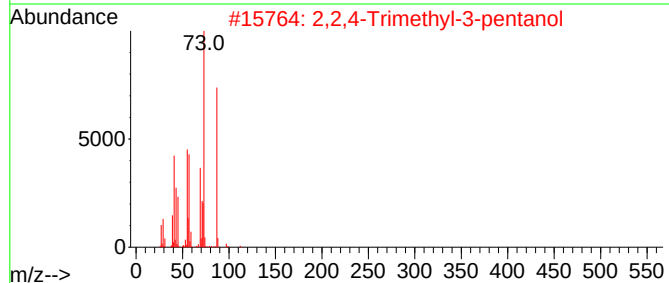
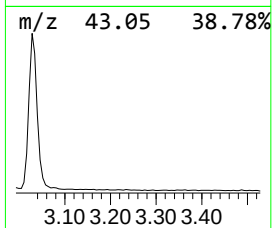
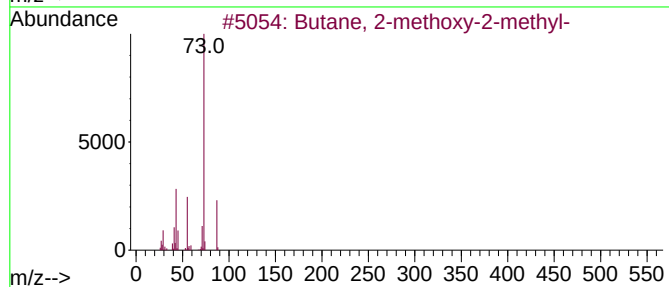
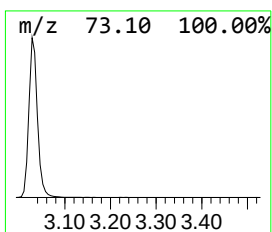
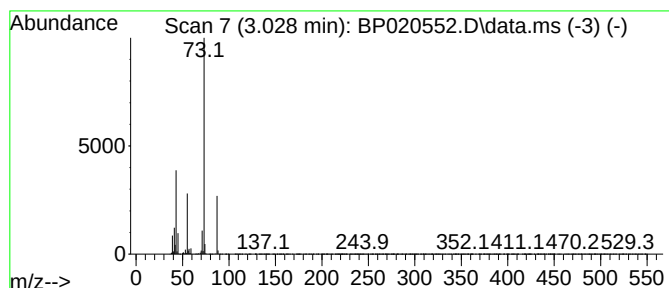
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	28.29 ng	2178360	1,4-Dichlorobenzene-d4	7.763

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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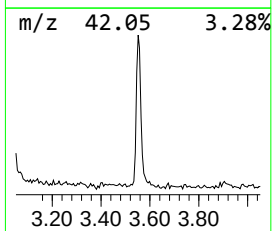
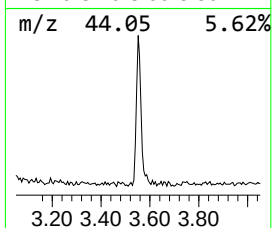
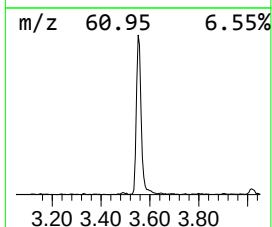
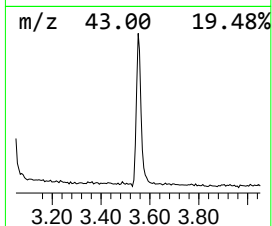
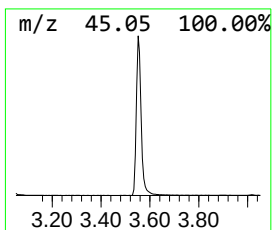
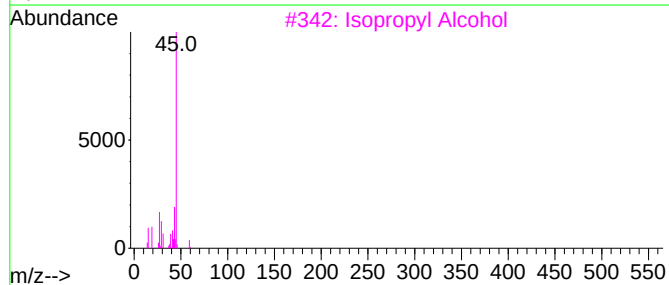
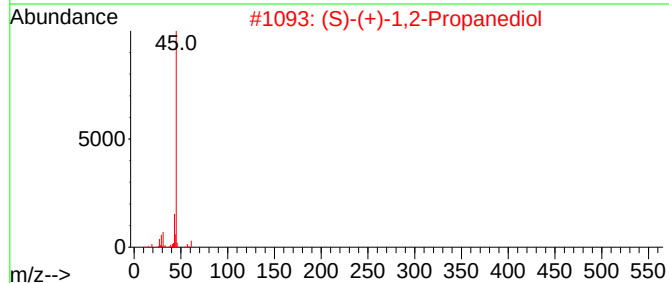
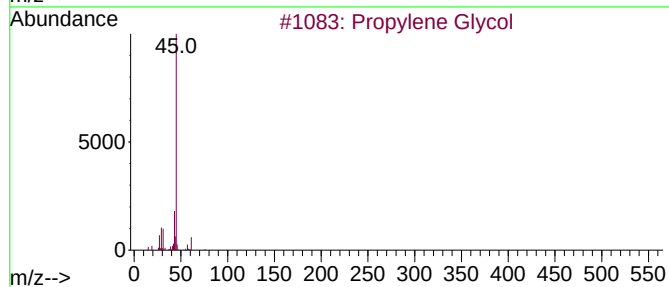
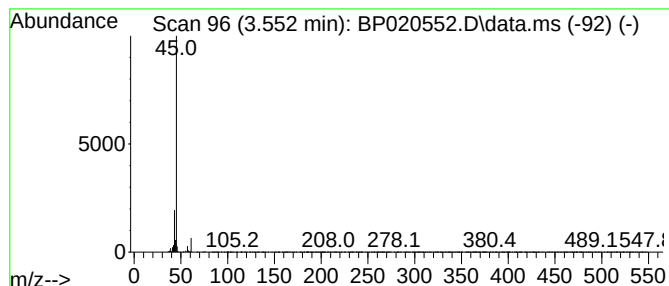
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.552	9.14 ng	703761	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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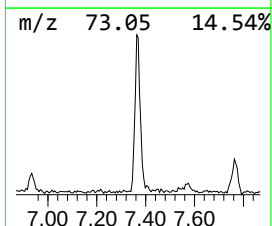
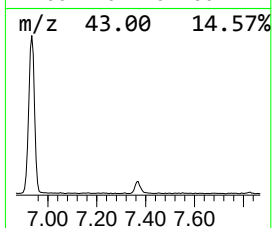
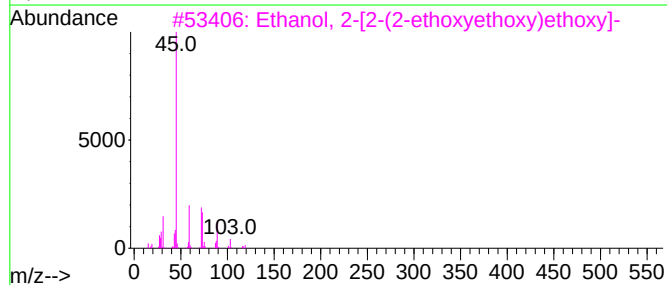
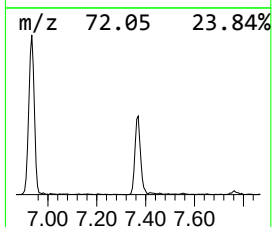
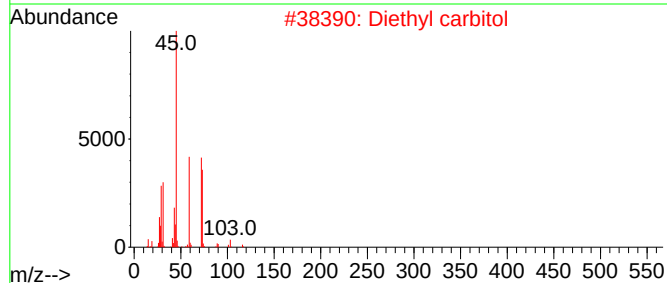
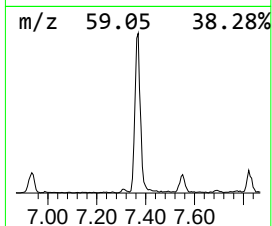
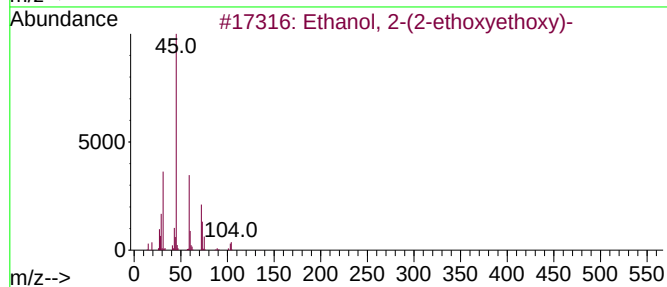
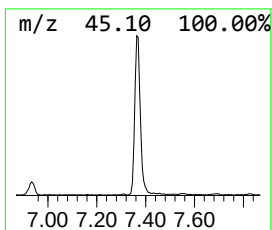
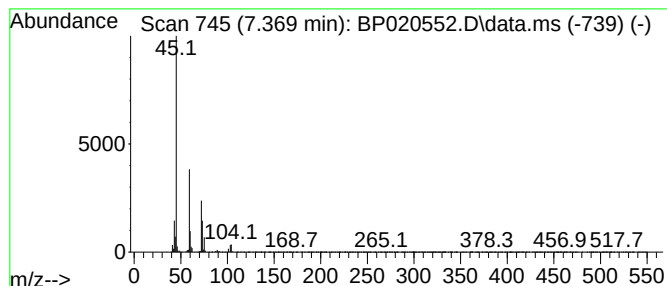
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.369	3.53 ng	271796	1,4-Dichlorobenzene-d4	7.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45
4			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45



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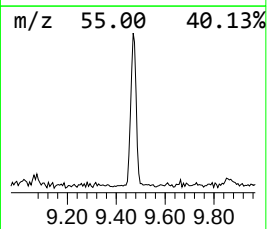
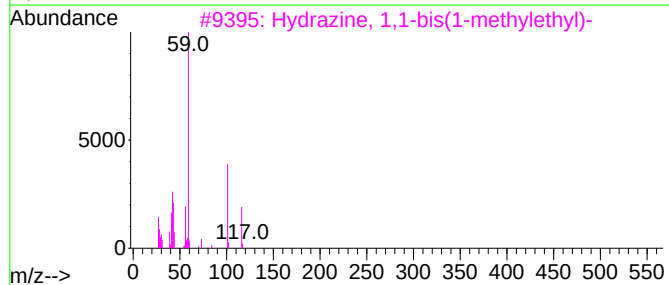
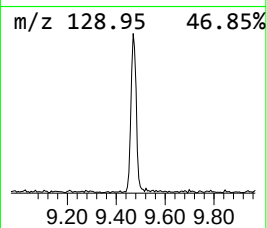
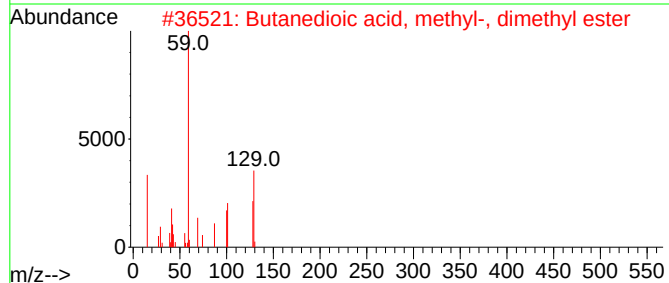
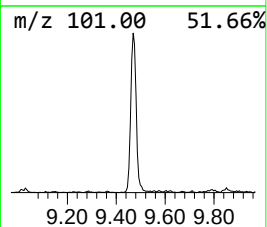
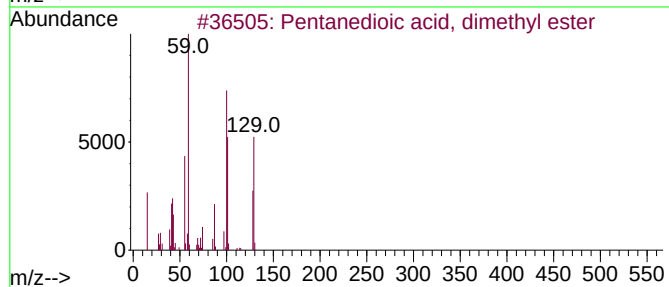
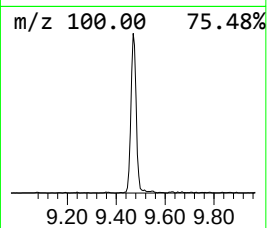
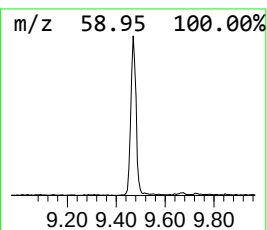
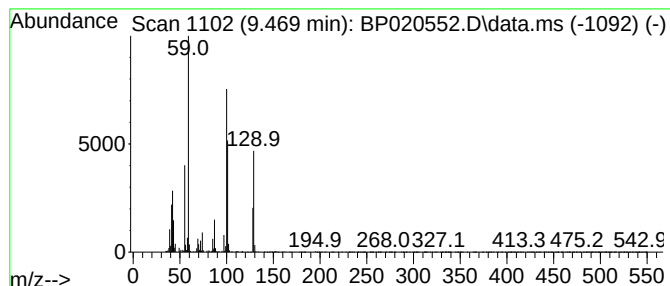
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentanedioic acid, dimethyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.469	2.04 ng	226640	Naphthalene-d8	10.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	43
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
4			Pyrrolidine, 1-nitroso-	100	C4H8N2O	000930-55-2	14
5			Piperazine, 2,5-dimethyl-3-propyl-	156	C9H20N2	054365-81-0	14



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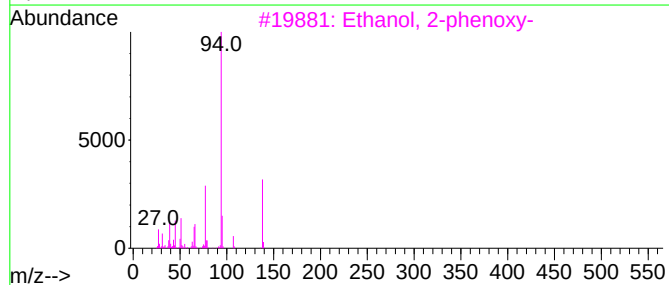
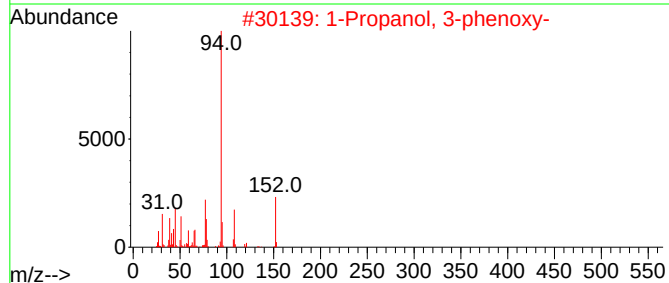
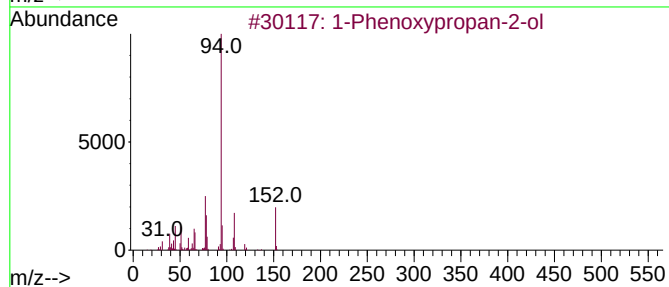
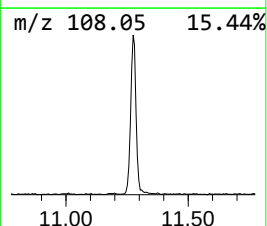
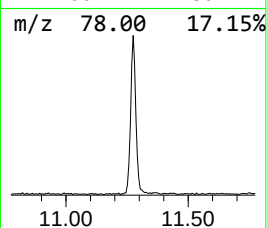
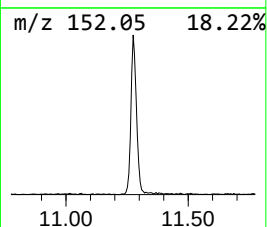
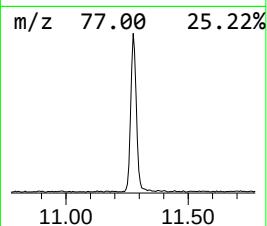
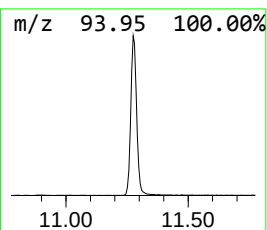
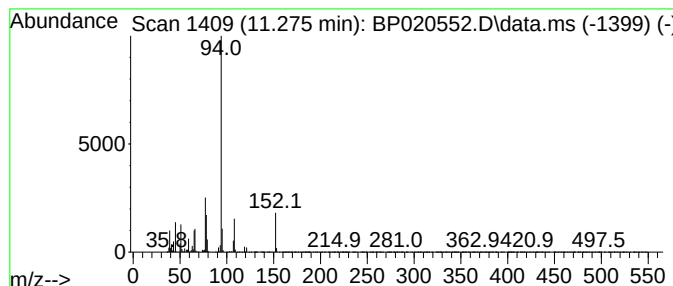
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.275	7.03 ng	781945	Naphthalene-d8	10.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			Benzene, (1,1-dimethylethoxy)-	150	C10H14O	006669-13-2	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060624\
Data File : BP020552.D
Acq On : 06 Jun 2024 22:44
Operator : MA/JU
Sample : P2715-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

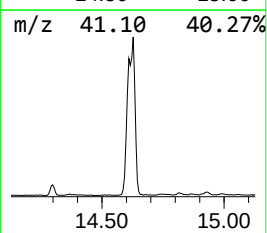
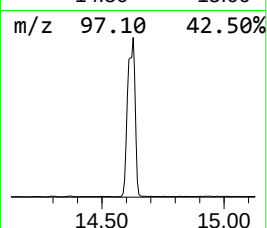
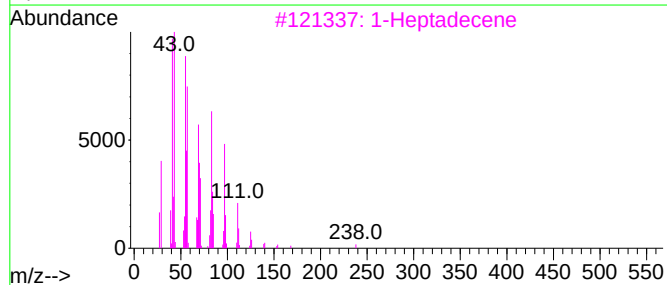
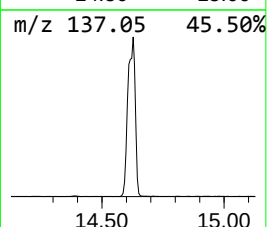
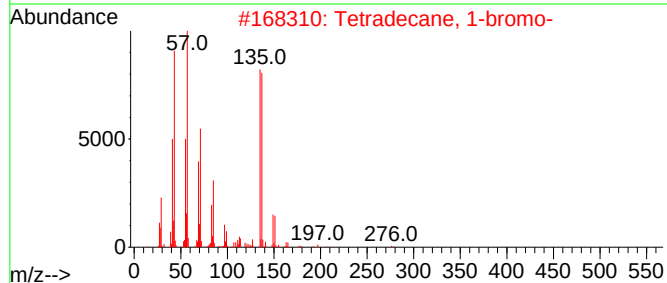
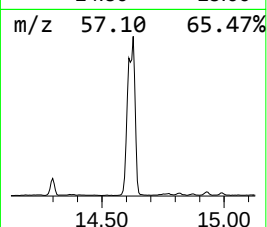
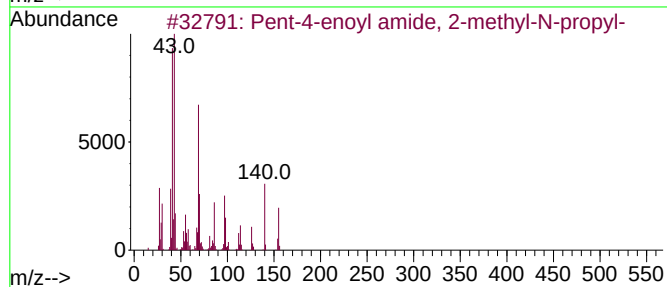
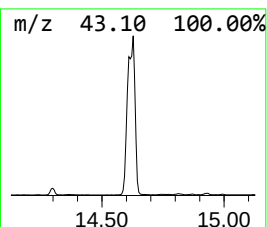
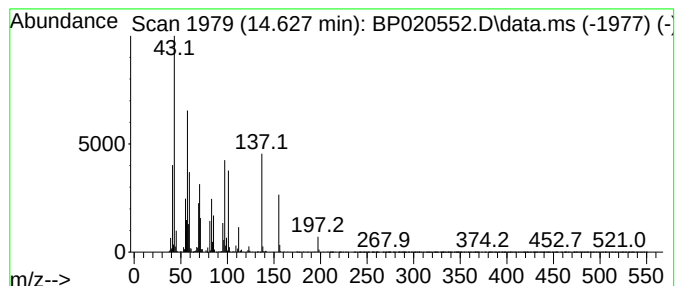
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ClientSampleId :
WCS-TPC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.628 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.628	27.87 ng	4138460	Acenaphthene-d10	14.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	27
2	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	14
3	1-Heptadecene	238	C17H34	006765-39-5	12
4	2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	11
5	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060624\
Data File : BP020552.D
Acq On : 06 Jun 2024 22:44
Operator : MA/JU
Sample : P2715-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPC

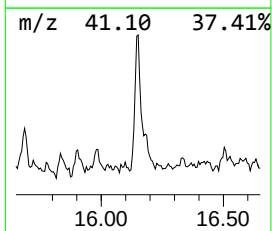
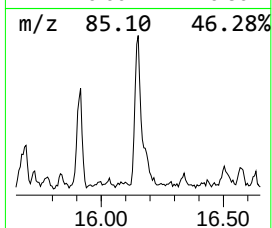
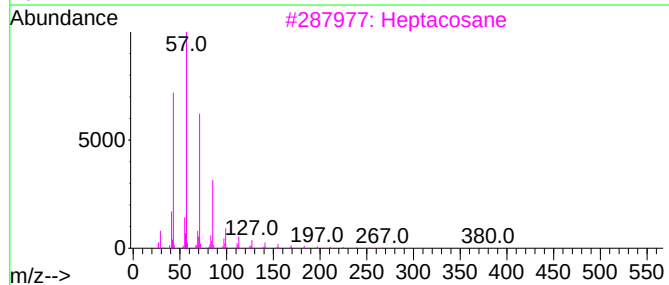
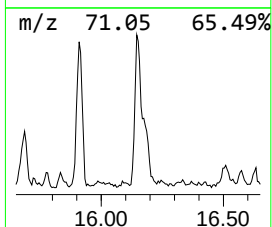
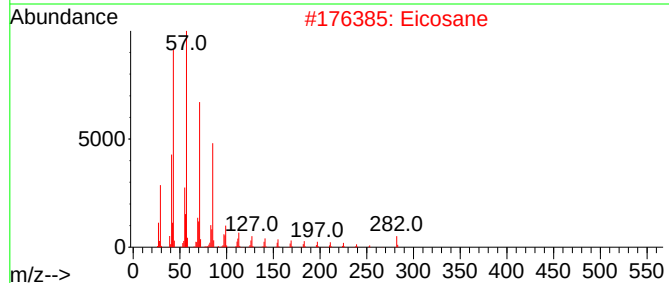
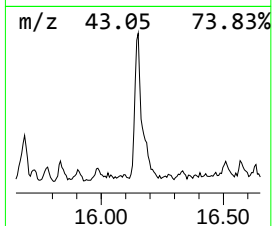
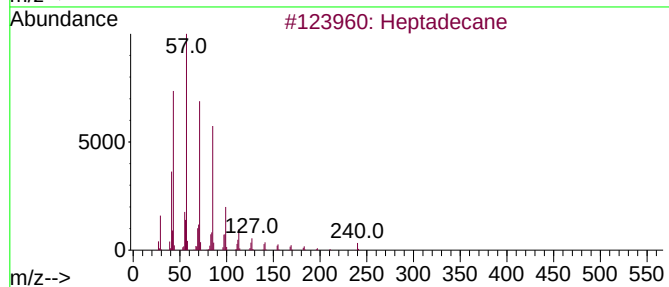
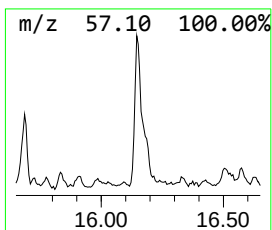
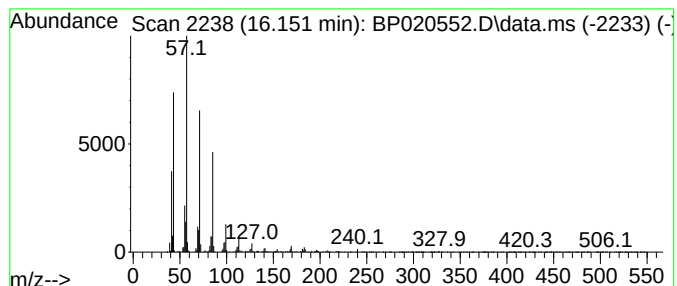
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.151	2.49 ng	421773	Phenanthrene-d10	17.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	97
2			Eicosane	282	C20H42	000112-95-8	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			Tridecane, 7-propyl-	226	C16H34	055045-09-5	91
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060624\
Data File : BP020552.D
Acq On : 06 Jun 2024 22:44
Operator : MA/JU
Sample : P2715-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPC

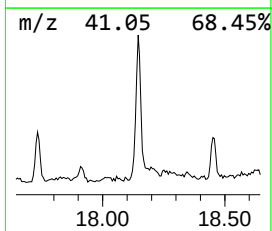
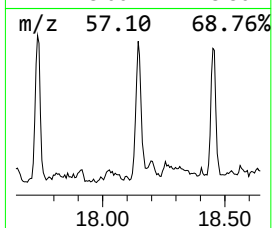
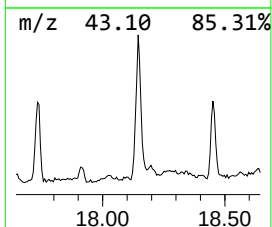
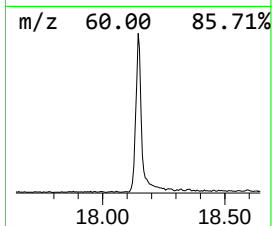
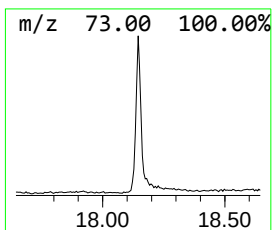
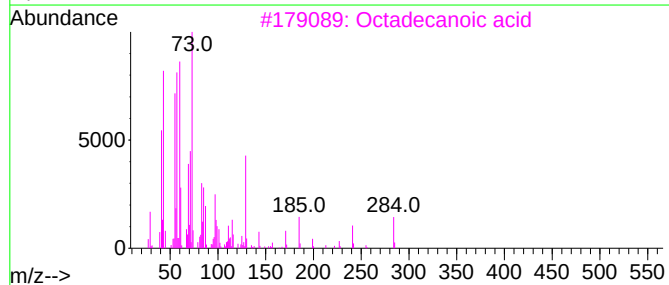
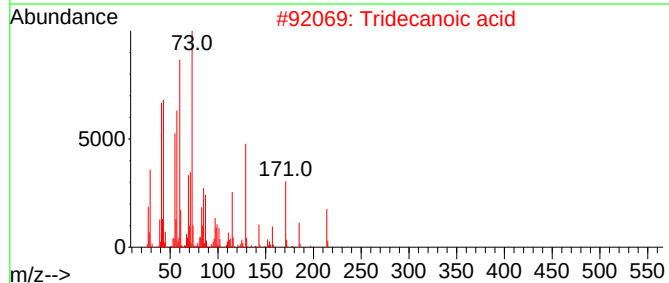
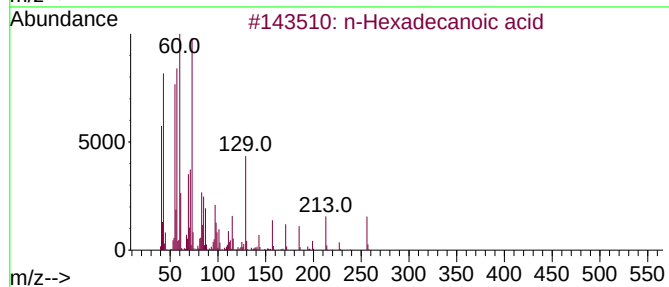
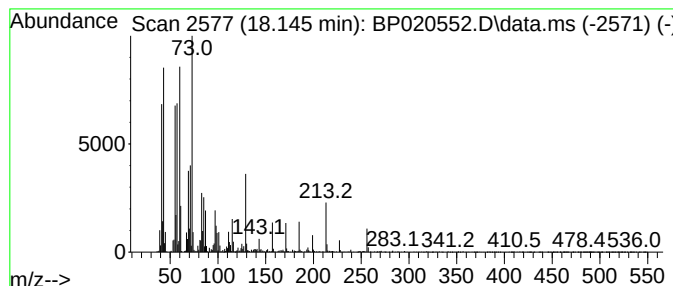
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	5.45 ng	924356	Phenanthrene-d10	17.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060624\
Data File : BP020552.D
Acq On : 06 Jun 2024 22:44
Operator : MA/JU
Sample : P2715-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WCS-TPC

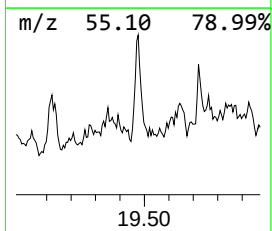
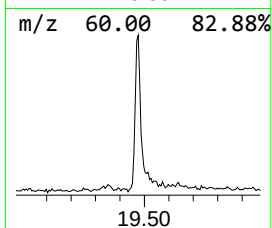
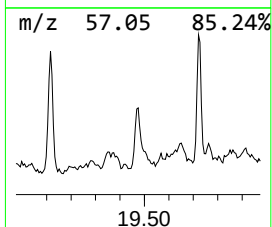
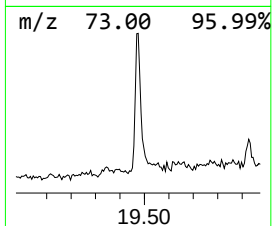
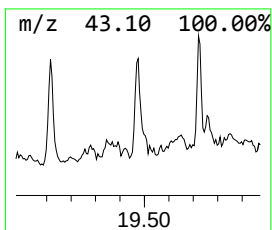
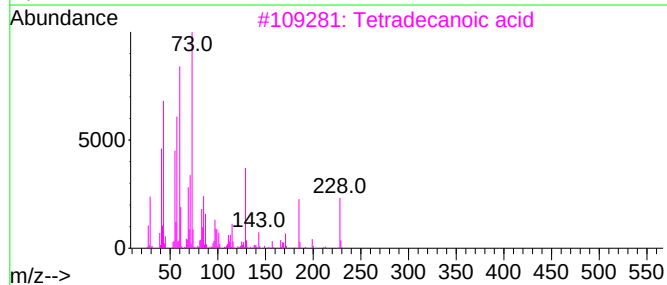
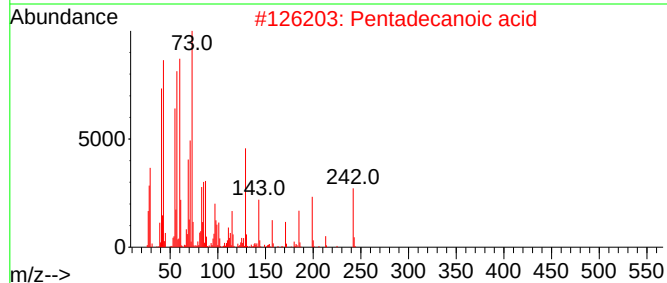
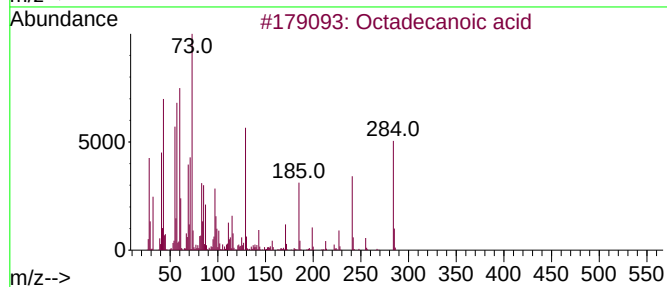
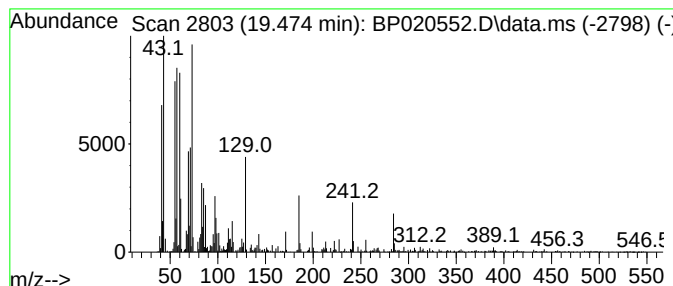
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.474	2.65 ng	440205	Chrysene-d12	21.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060624\
Data File : BP020552.D
Acq On : 06 Jun 2024 22:44
Operator : MA/JU
Sample : P2715-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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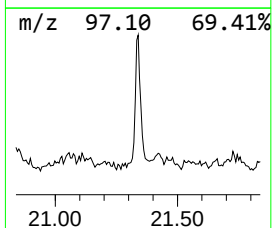
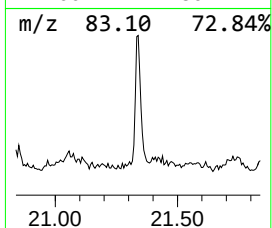
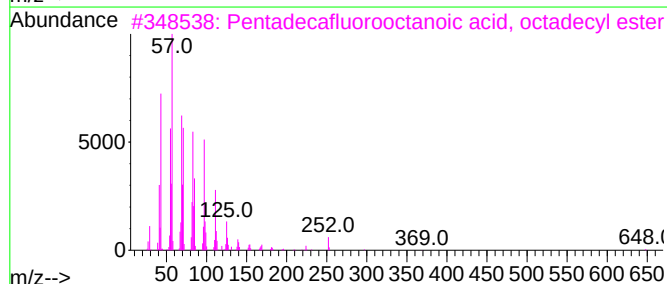
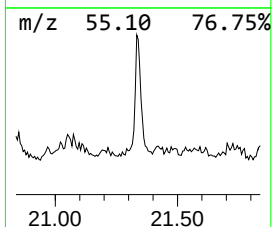
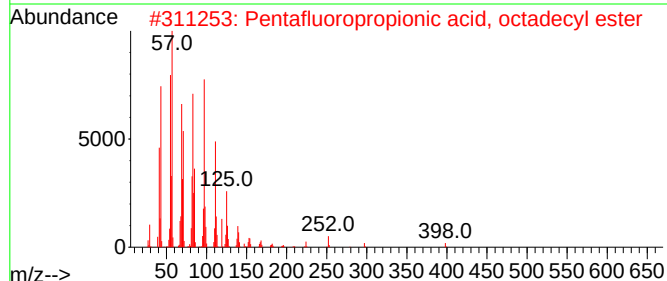
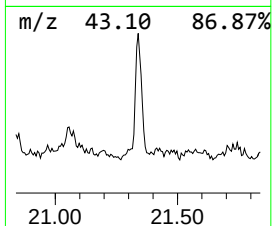
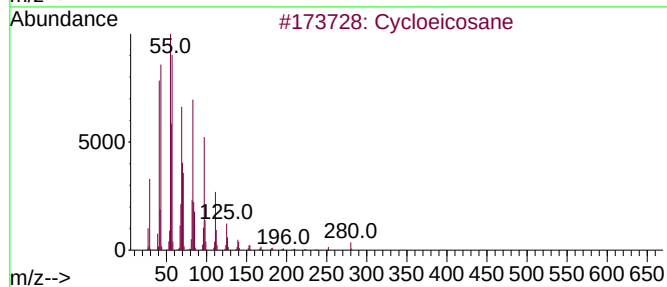
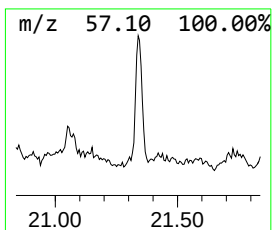
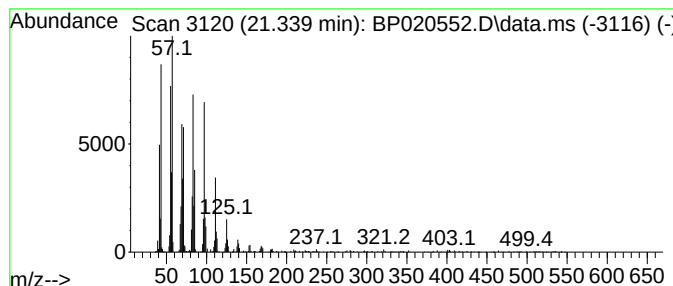
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cycloeicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.339	5.83 ng	969511	Chrysene-d12	21.657

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloeicosane	280	C20H40	000296-56-0	96
2		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	94
3		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4		1-Triacontanol	438	C30H62O	000593-50-0	94
5		1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060624\
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Acq On : 06 Jun 2024 22:44
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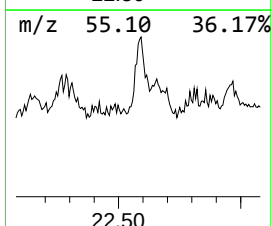
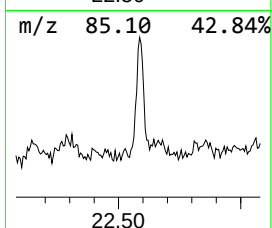
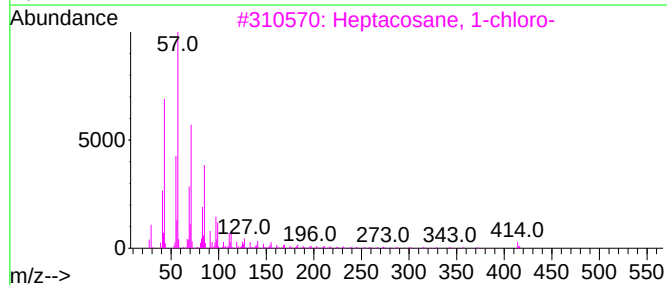
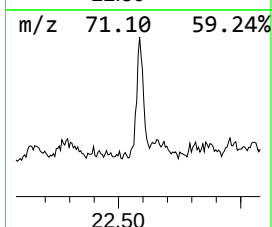
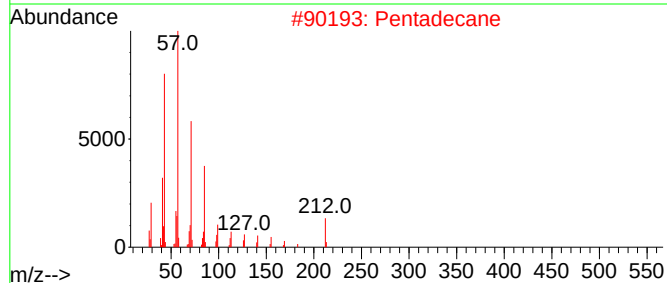
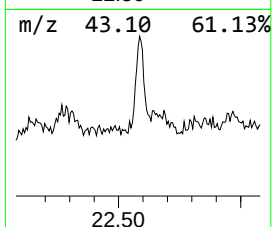
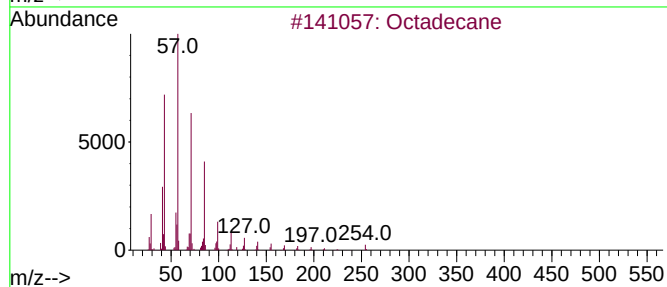
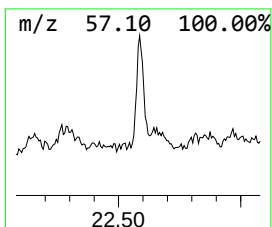
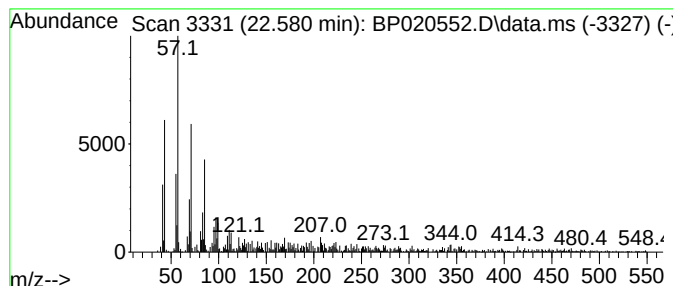
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.580	3.32 ng	552393	Chrysene-d12	21.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	97
2			Pentadecane	212	C15H32	000629-62-9	95
3			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	94
4			Nonadecane	268	C19H40	000629-92-5	94
5			Pentacosane	352	C25H52	000629-99-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060624\
Data File : BP020552.D
Acq On : 06 Jun 2024 22:44
Operator : MA/JU
Sample : P2715-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPC

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.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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Propylene Glycol	3.552	9.1	ng	703761	1	7.763	1539830	20.0
Ethanol, 2-(2-e...	7.369	3.5	ng	271796	1	7.763	1539830	20.0
Pentanedioic ac...	9.469	2.0	ng	226640	2	10.540	2223200	20.0
1-Phenoxypropan...	11.275	7.0	ng	781945	2	10.540	2223200	20.0
unknown14.628	14.628	27.9	ng	4138460	3	14.392	2970110	20.0
Heptadecane	16.151	2.5	ng	421773	4	17.198	3389470	20.0
n-Hexadecanoic ...	18.145	5.5	ng	924356	4	17.198	3389470	20.0
Octadecanoic acid	19.474	2.6	ng	440205	5	21.657	3327580	20.0
Cycloeicosane	21.339	5.8	ng	969511	5	21.657	3327580	20.0
Octadecane	22.580	3.3	ng	552393	5	21.657	3327580	20.0