

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041524\
 Data File : BG060903.D
 Acq On : 15 Apr 2024 16:25
 Operator : MA/JU
 Sample : P2114-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NB-08-041224

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_G\Methods\8270-BG032924.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060903.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.170	26	31	46	rVB	92445	182033	4.82%	0.864%
2	3.687	114	119	129	rBV	37878	66338	1.76%	0.315%
3	5.538	426	434	447	rBV	1131490	1865055	49.42%	8.848%
4	7.112	693	702	715	rBV	1137354	1961517	51.97%	9.305%
5	7.947	838	844	850	rBV	220912	367504	9.74%	1.743%
6	9.098	1031	1040	1049	rBV	715789	1257395	33.32%	5.965%
7	10.514	1274	1281	1290	rBV2	34748	61446	1.63%	0.292%
8	10.743	1312	1320	1327	rBV	309437	561760	14.88%	2.665%
9	11.948	1517	1525	1531	rVB	74110	119660	3.17%	0.568%
10	12.177	1558	1564	1570	rBV	57872	83608	2.22%	0.397%
11	12.383	1593	1599	1607	rVB	282316	462142	12.25%	2.192%
12	12.641	1634	1643	1650	rVB2	31028	62375	1.65%	0.296%
13	13.199	1731	1738	1749	rBV	1517790	2449474	64.90%	11.620%
14	13.417	1767	1775	1783	rBV	57394	91395	2.42%	0.434%
15	14.574	1965	1972	1979	rBV	501497	781552	20.71%	3.708%
16	16.061	2218	2225	2236	rBV	1481216	2373097	62.88%	11.258%
17	16.302	2262	2266	2270	rBV2	27414	40268	1.07%	0.191%
18	17.101	2397	2402	2406	rBV	32937	40825	1.08%	0.194%
19	17.324	2434	2440	2445	rBV	675250	997593	26.43%	4.733%
20	17.723	2500	2508	2520	rBV4	27428	65196	1.73%	0.309%
21	18.229	2589	2594	2602	rBV	230712	341429	9.05%	1.620%
22	18.663	2664	2668	2671	rBV2	38605	45623	1.21%	0.216%
23	19.163	2748	2753	2763	rVB6	33864	84389	2.24%	0.400%
24	19.380	2784	2790	2793	rBV	64495	98274	2.60%	0.466%
25	19.504	2807	2811	2820	rBV2	91698	146663	3.89%	0.696%
26	19.739	2842	2851	2855	rBV3	86492	139468	3.70%	0.662%
27	19.944	2878	2886	2893	rBV	2774163	3774055	100.00%	17.904%
28	20.273	2938	2942	2947	rVB	32180	45283	1.20%	0.215%
29	21.266	3106	3111	3117	rBV2	136464	240143	6.36%	1.139%
30	21.584	3158	3165	3171	rBV2	694666	1137027	30.13%	5.394%
31	21.813	3201	3204	3209	rVB3	38718	50115	1.33%	0.238%
32	24.721	3690	3699	3707	rVB	393002	1086516	28.79%	5.154%

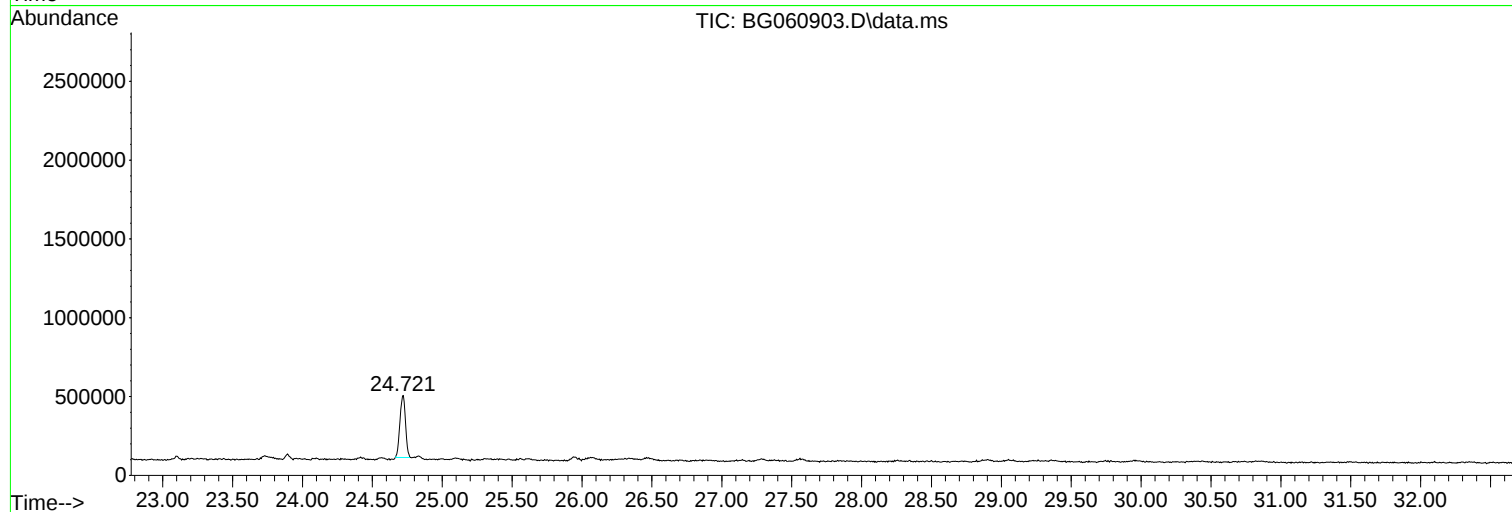
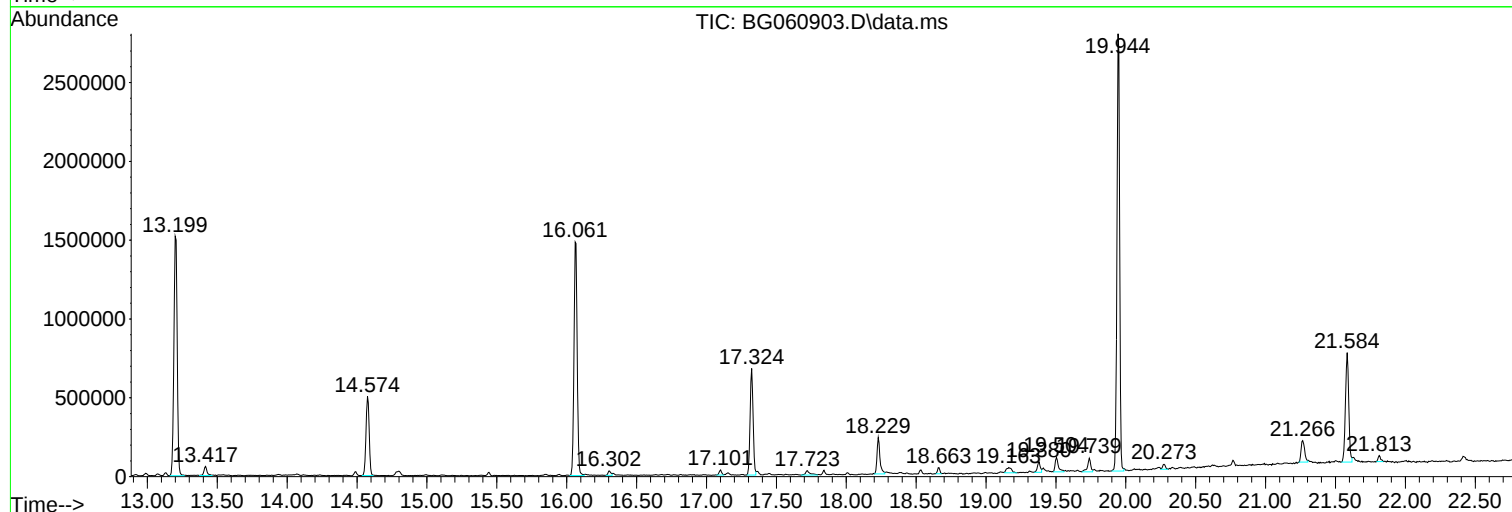
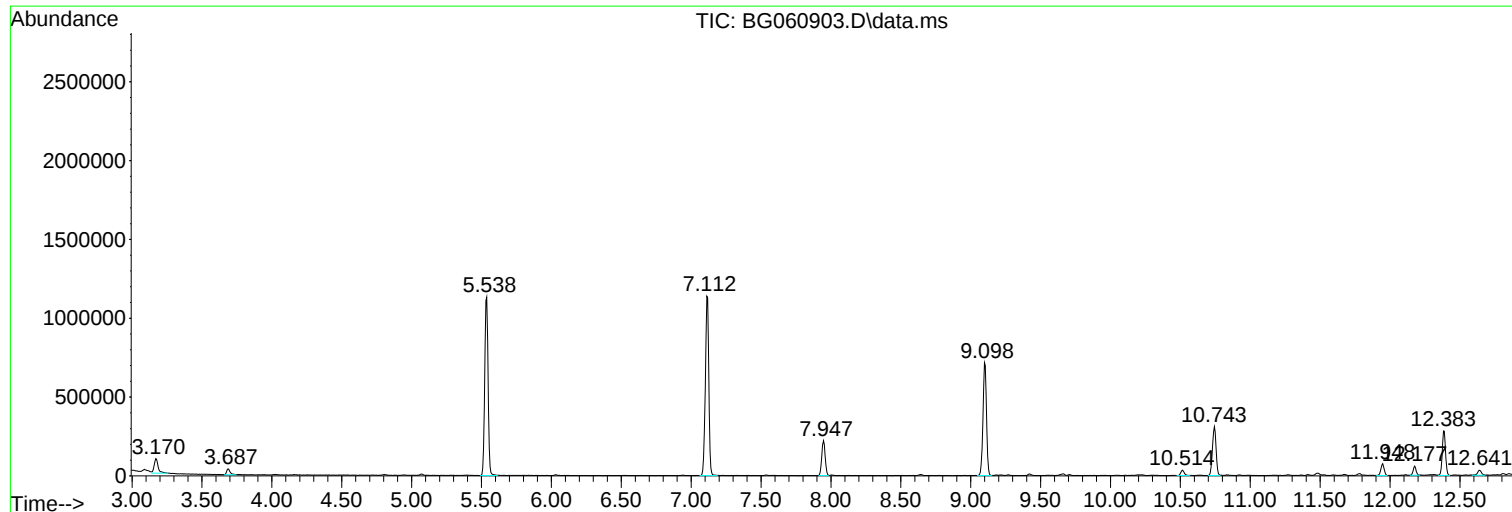
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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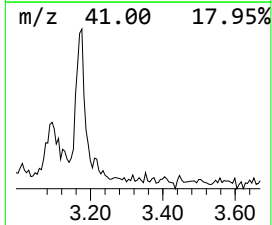
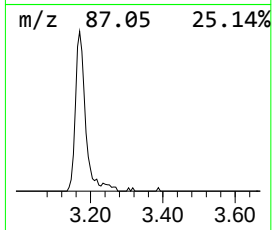
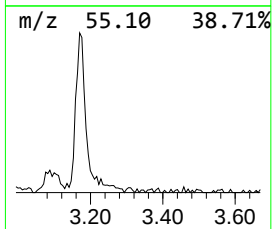
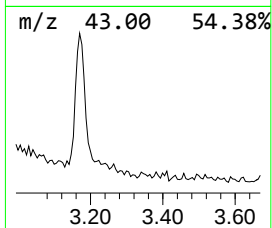
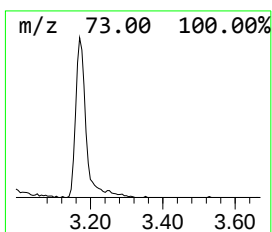
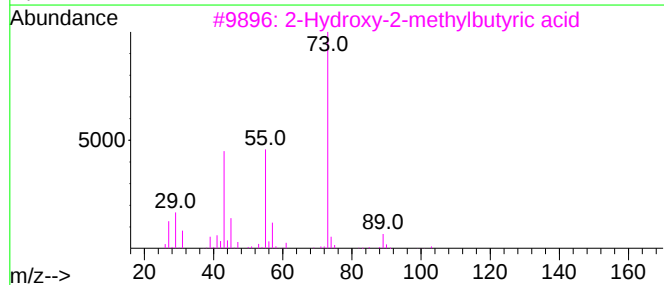
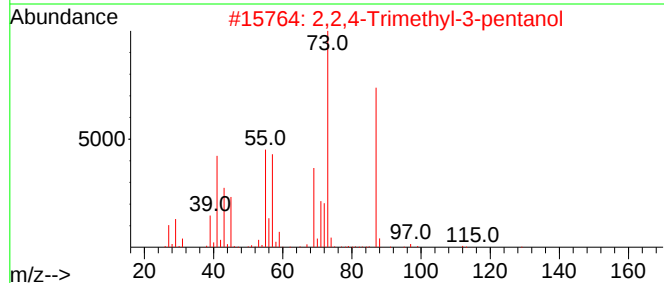
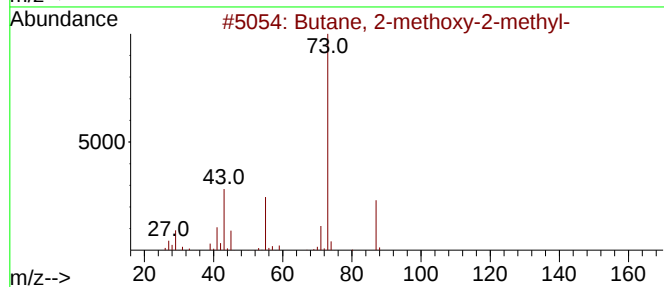
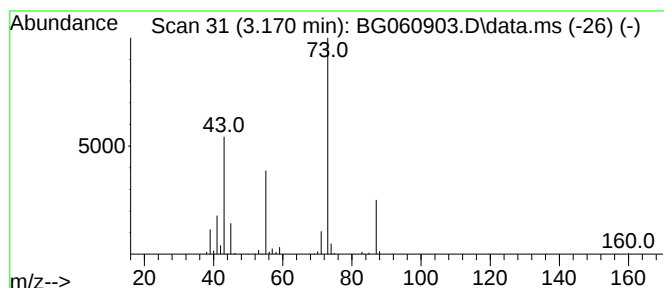
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.170	9.91 ng	182033	1,4-Dichlorobenzene-d4	7.947

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	38
3			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	28
4			Pentanoic acid, 2-hydroxy-4-meth...	146	C7H14O3	040348-72-9	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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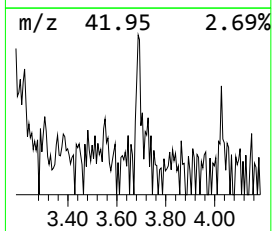
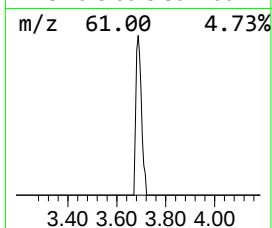
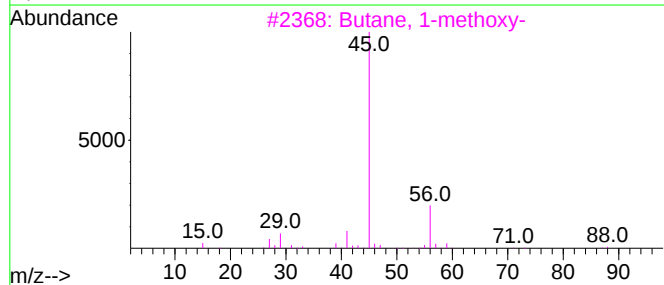
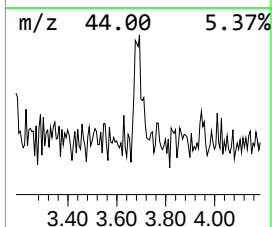
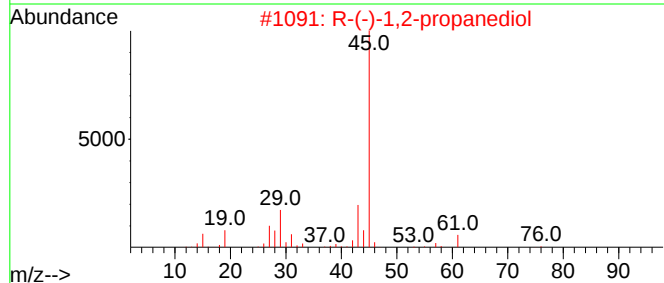
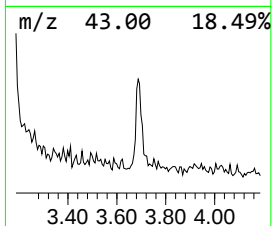
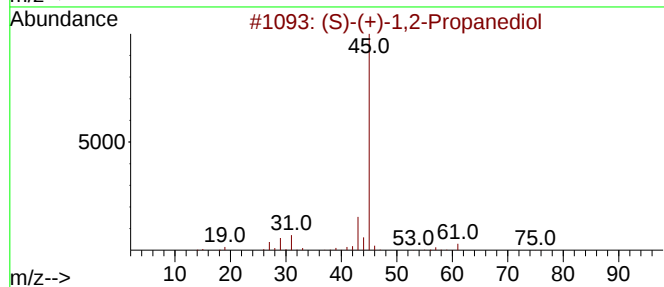
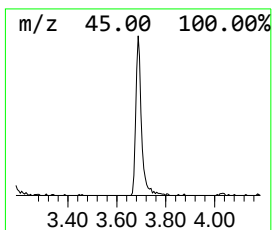
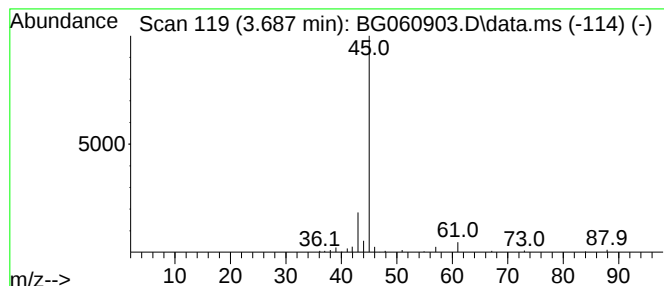
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.687	3.61 ng	66338	1,4-Dichlorobenzene-d4	7.947

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	56
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	40
3	Butane, 1-methoxy-			88	C5H12O	000628-28-4	9
4	Propylene Glycol			76	C3H8O2	000057-55-6	9
5	Propanal, 3-methoxy-			88	C4H8O2	002806-84-0	7



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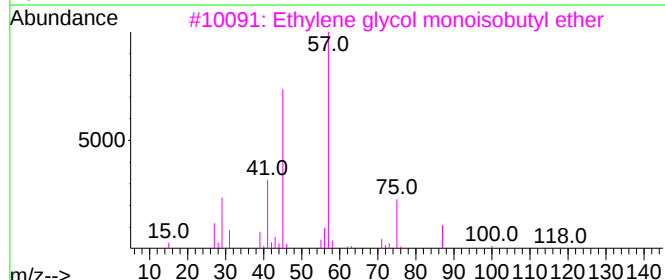
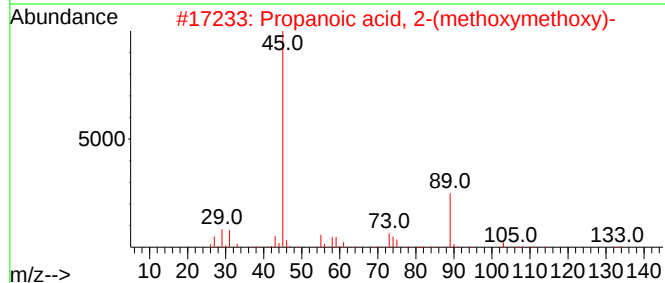
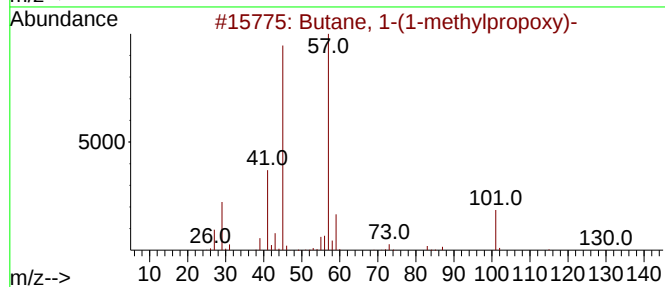
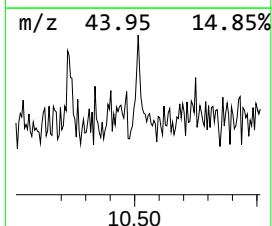
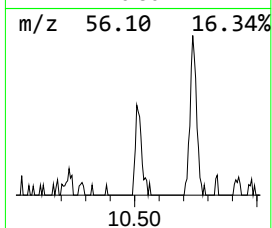
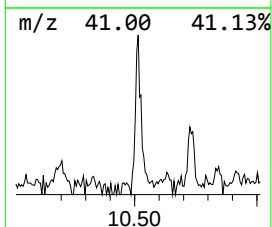
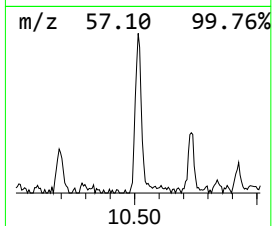
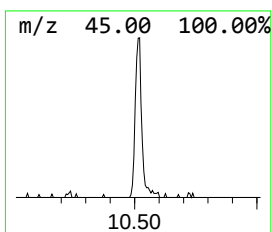
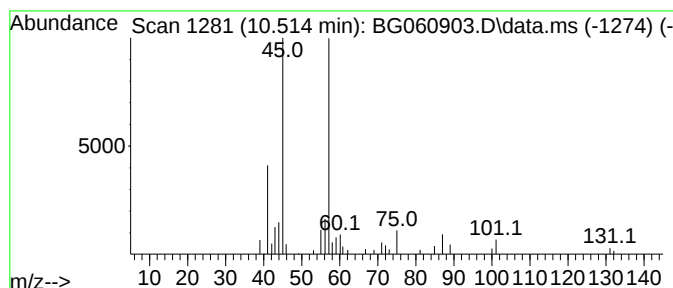
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 1-(1-methylpropoxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.514	2.19 ng	61446	Naphthalene-d8	10.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
2			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
4			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	43
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	39



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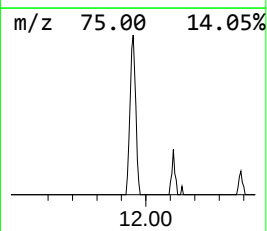
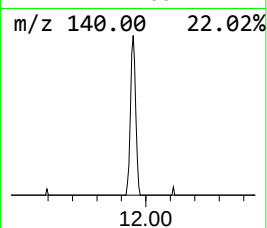
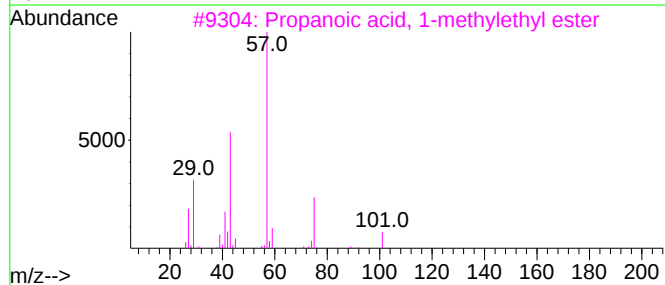
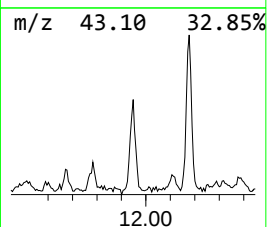
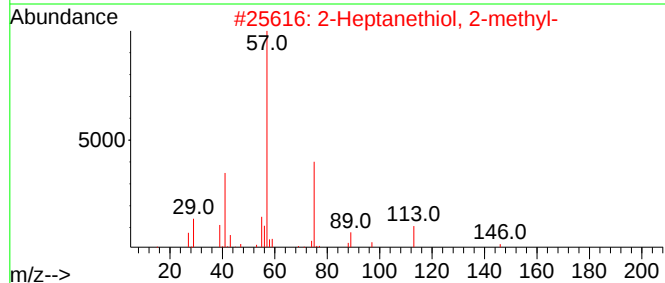
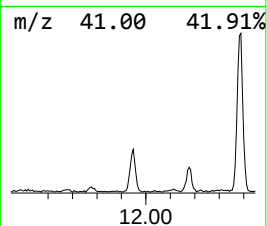
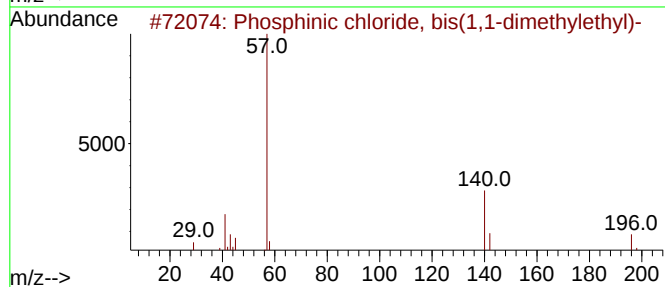
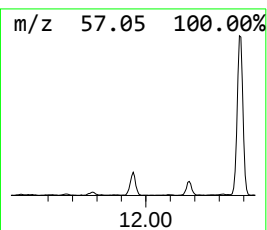
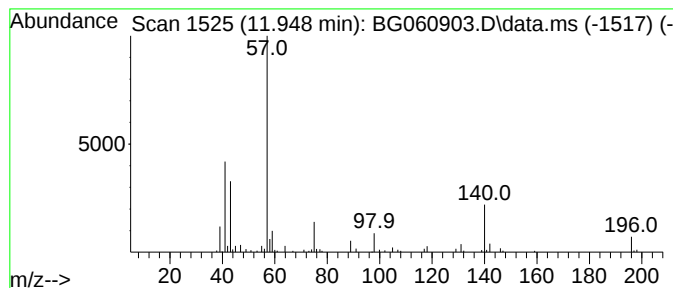
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Peak Number 4 unknown11.948 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.948	4.26 ng	119660	Naphthalene-d8	10.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphinic chloride, bis(1,1-dim...	196	C8H18ClOP	000677-74-7	37
2			2-Heptanethiol, 2-methyl-	146	C8H18S	000763-20-2	16
3			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	10
4			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	10
5			tert-Butyl N-(tert-butoxy)carbamate	189	C9H19NO3	091426-13-0	9



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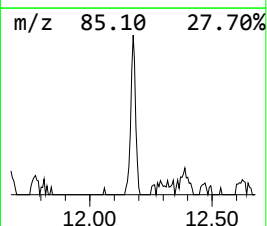
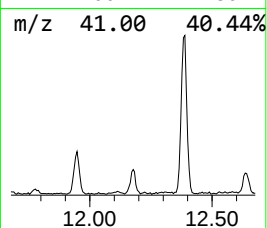
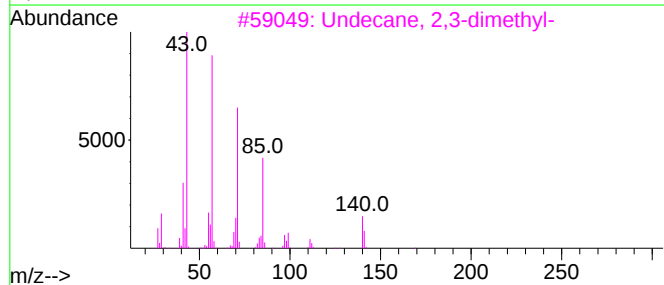
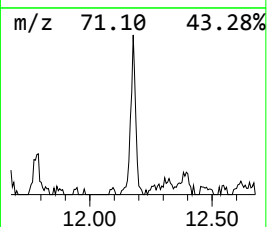
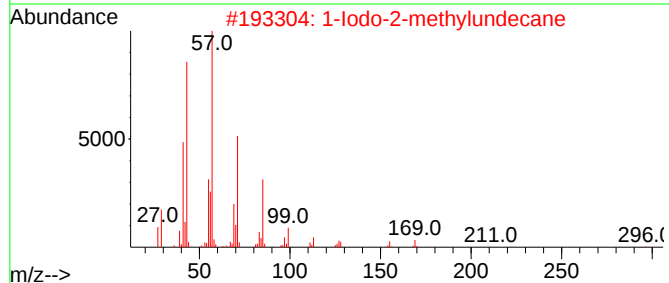
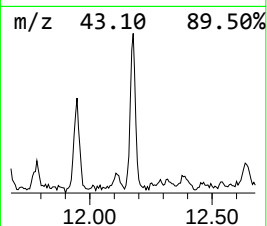
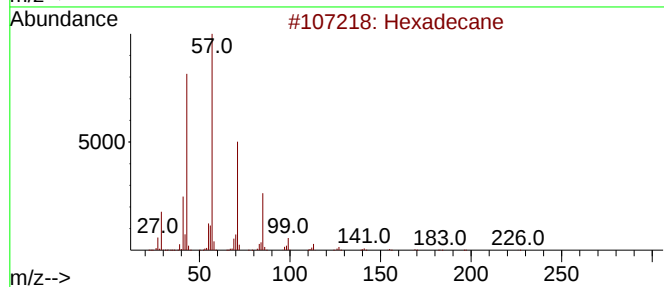
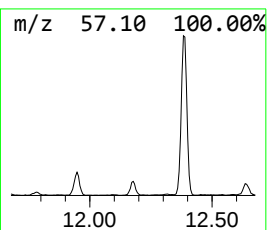
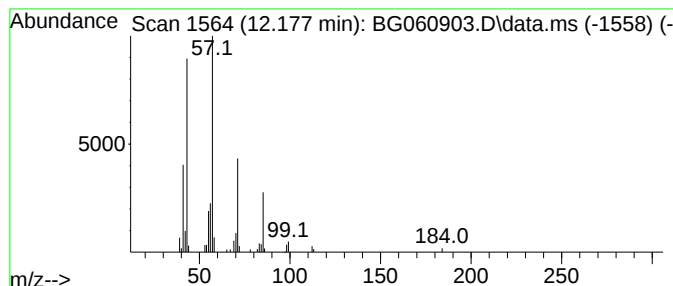
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Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.177	2.98 ng	83608	Naphthalene-d8	10.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	86
2			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83
3			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	64
4			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59
5			Tridecane	184	C13H28	000629-50-5	58



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ClientSampleId :
NB-08-041224

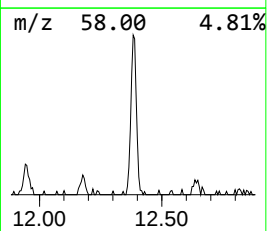
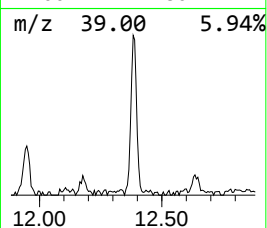
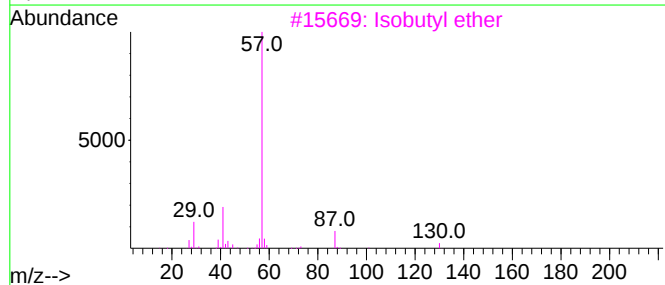
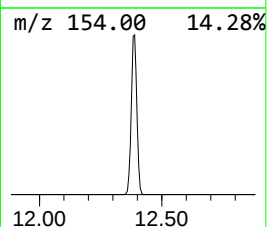
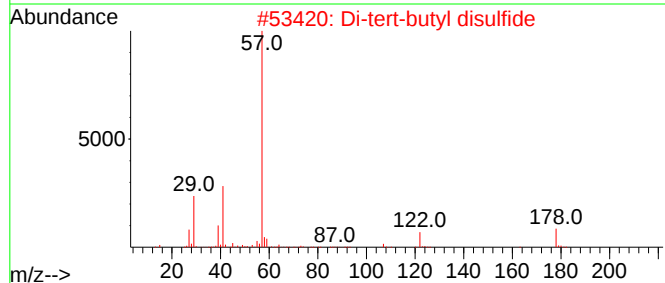
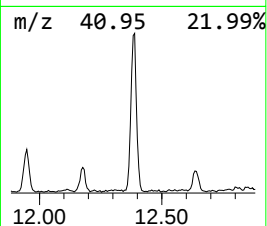
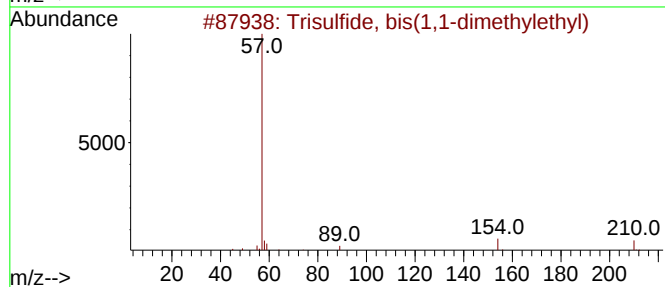
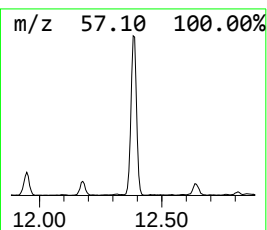
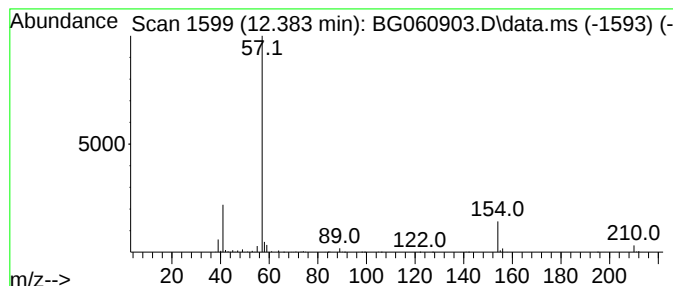
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown12.383 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.383	16.45 ng	462142	Naphthalene-d8	10.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	45
2			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	28
3			Isobutyl ether	130	C8H18O	000628-55-7	25
4			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	9
5			Hypophosphonous dichloride, bis(...	246	C8H18Cl2P2	079898-85-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041524\
Data File : BG060903.D
Acq On : 15 Apr 2024 16:25
Operator : MA/JU
Sample : P2114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NB-08-041224

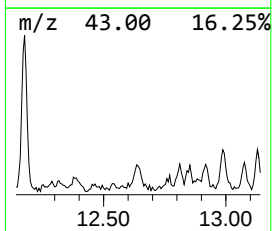
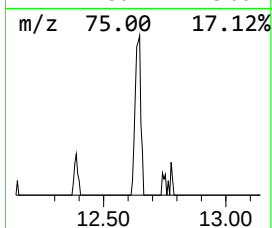
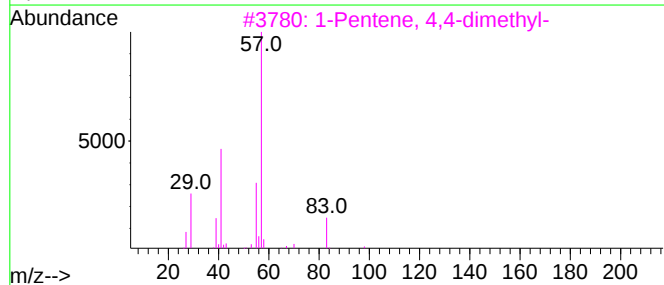
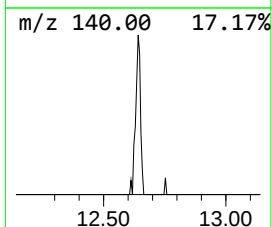
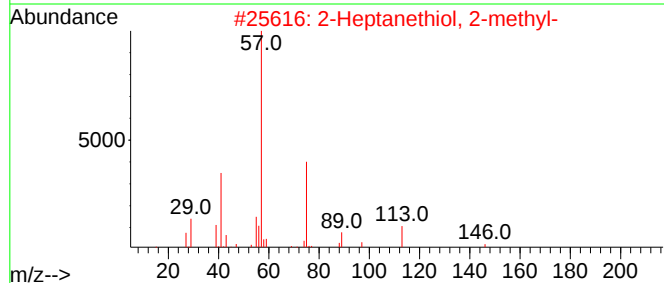
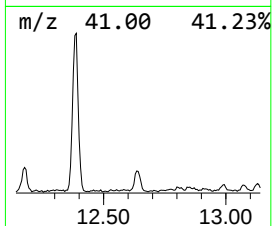
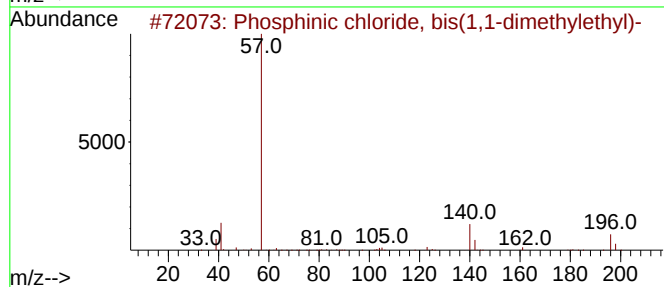
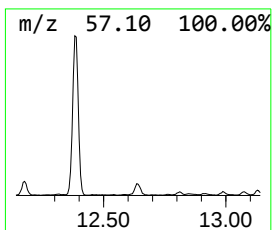
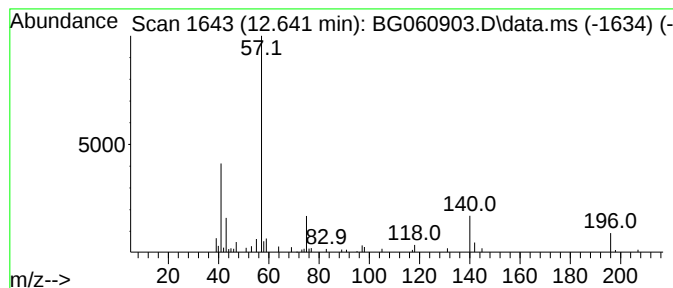
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.641 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.641	2.22 ng	62375	Naphthalene-d8	10.743

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphinic chloride, bis(1,1-dim...	196	C8H18ClOP	000677-74-7	47
2			2-Heptanethiol, 2-methyl-	146	C8H18S	000763-20-2	17
3			1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	10
4			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	10
5			Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041524\
Data File : BG060903.D
Acq On : 15 Apr 2024 16:25
Operator : MA/JU
Sample : P2114-01
Misc :
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Instrument :
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ClientSampleId :
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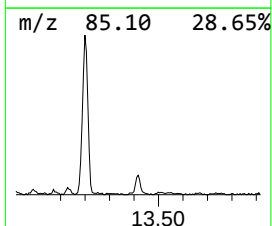
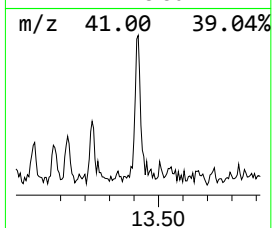
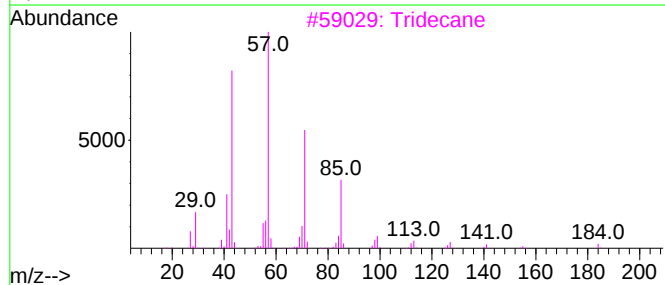
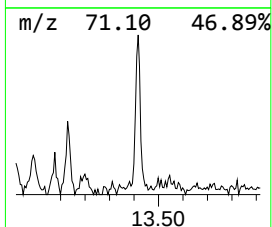
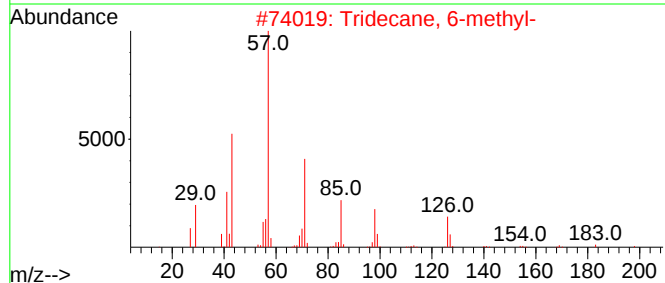
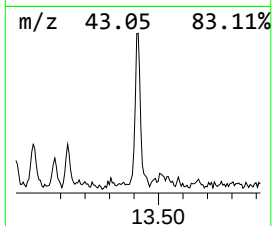
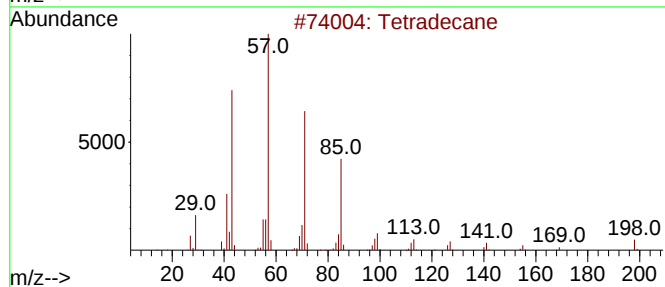
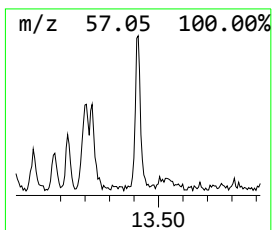
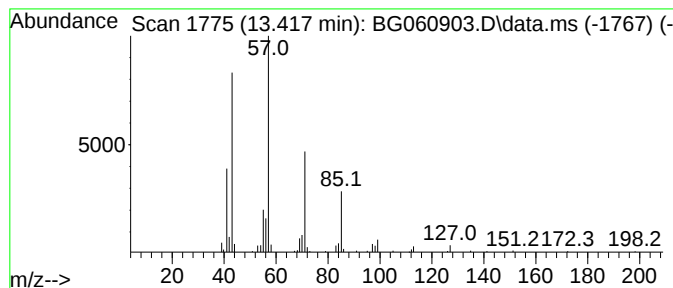
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.417	2.34 ng	91395	Acenaphthene-d10	14.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	90
2			Tridecane, 6-methyl-	198	C14H30	013287-21-3	87
3			Tridecane	184	C13H28	000629-50-5	86
4			Heptadecane	240	C17H36	000629-78-7	86
5			Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041524\
Data File : BG060903.D
Acq On : 15 Apr 2024 16:25
Operator : MA/JU
Sample : P2114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NB-08-041224

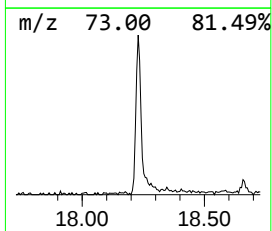
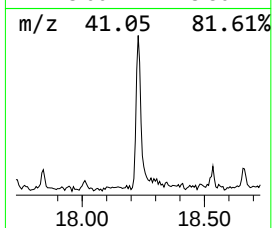
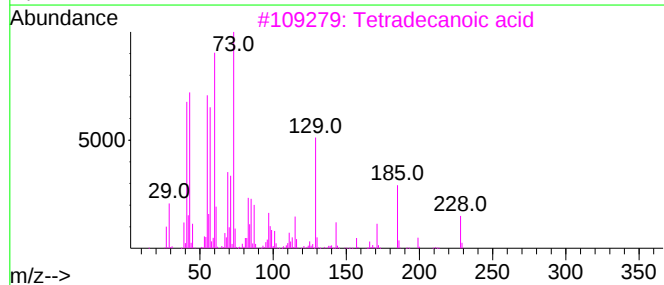
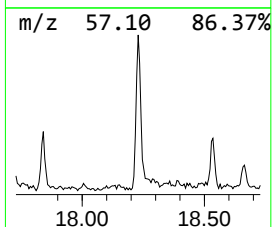
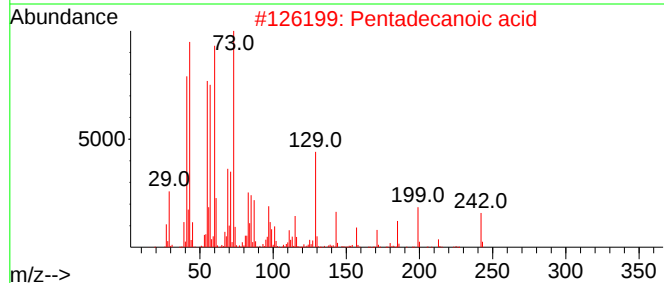
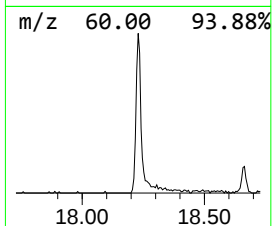
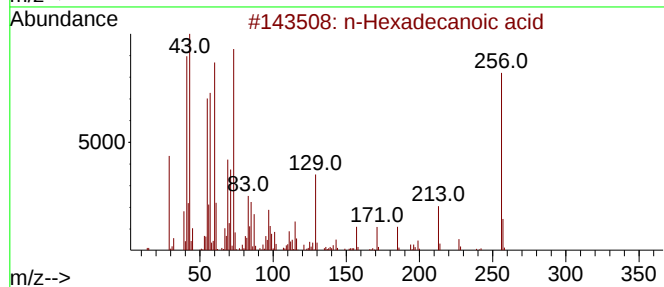
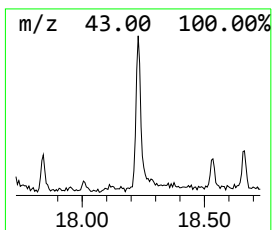
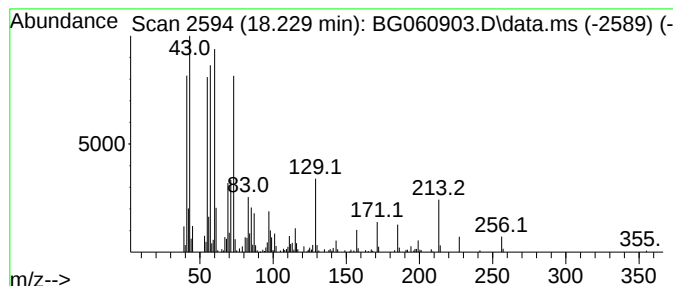
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.229	6.85 ng	341429	Phenanthrene-d10	17.324

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041524\
Data File : BG060903.D
Acq On : 15 Apr 2024 16:25
Operator : MA/JU
Sample : P2114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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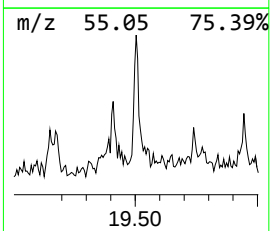
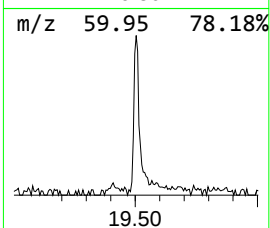
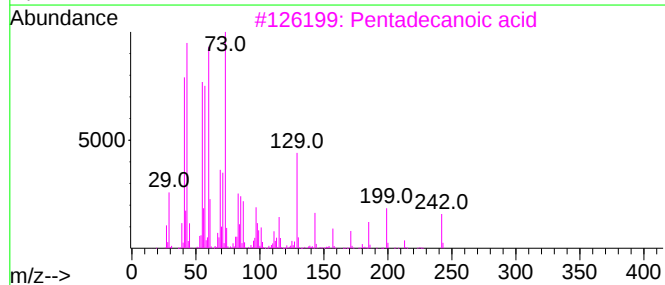
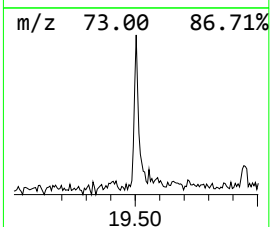
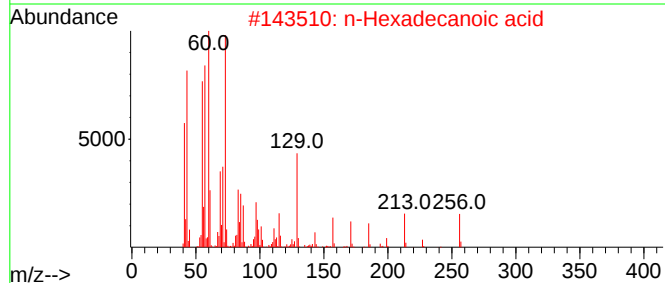
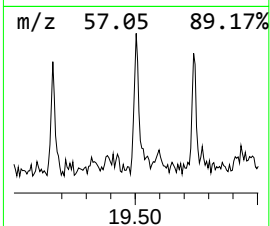
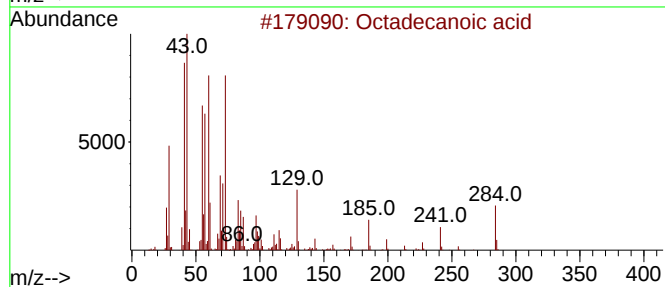
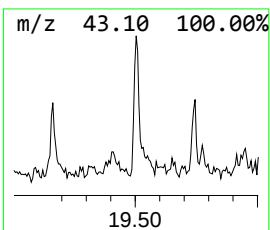
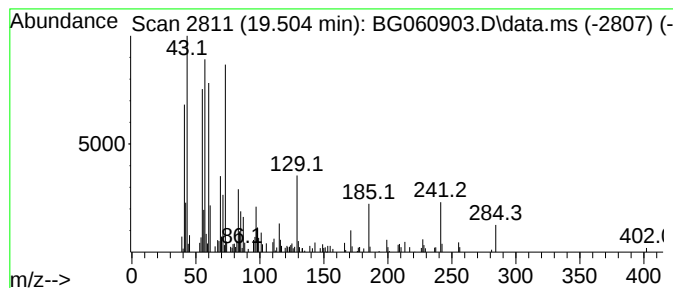
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.504	2.58 ng	146663	Chrysene-d12	21.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041524\
Data File : BG060903.D
Acq On : 15 Apr 2024 16:25
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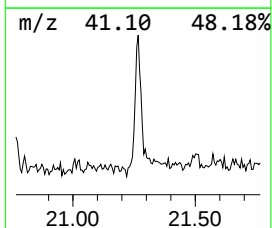
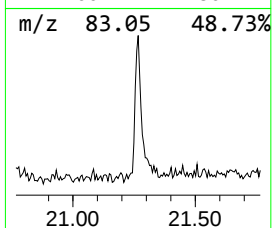
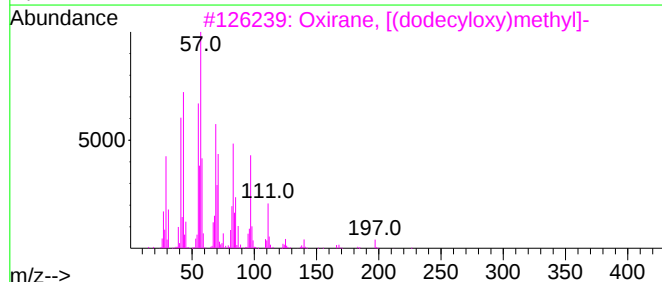
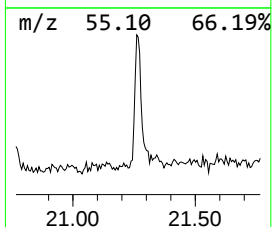
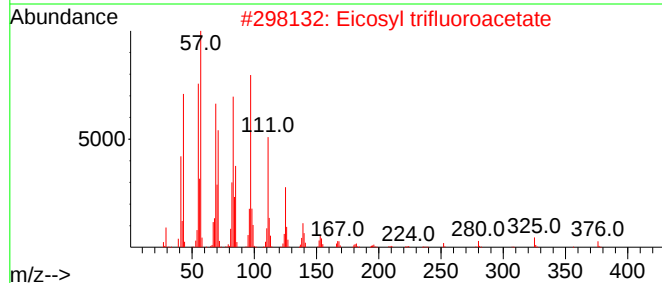
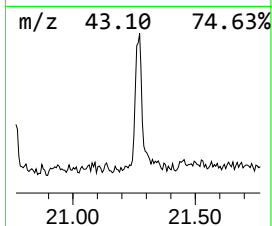
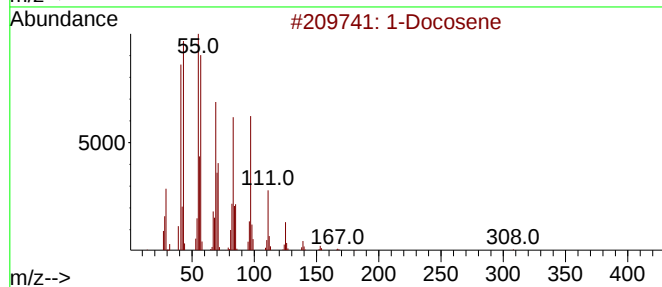
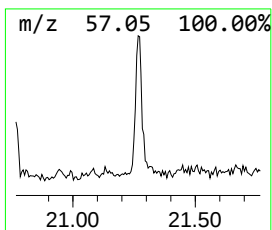
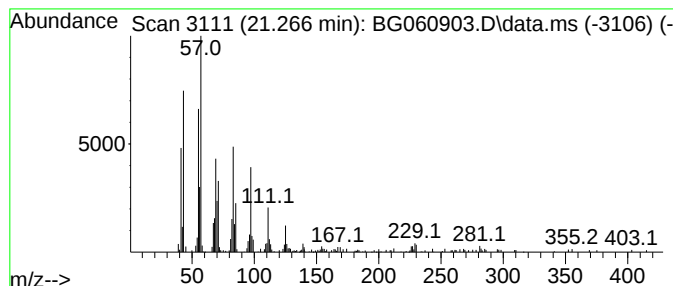
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.266	4.22 ng	240143	Chrysene-d12	21.584

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	93
2			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91
3			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	91
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Heneicosyl trifluoroacetate	408	C23H43F3O2	1000351-76-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041524\
Data File : BG060903.D
Acq On : 15 Apr 2024 16:25
Operator : MA/JU
Sample : P2114-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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

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

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					#	RT	Resp	Conc
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(S)-(+)-1,2-Pro...	3.687	3.6	ng	66338	1	7.947	367504	20.0
Butane, 1-(1-me...	10.514	2.2	ng	61446	2	10.743	561760	20.0
unknown11.948	11.948	4.3	ng	119660	2	10.743	561760	20.0
Hexadecane	12.177	3.0	ng	83608	2	10.743	561760	20.0
unknown12.383	12.383	16.4	ng	462142	2	10.743	561760	20.0
unknown12.641	12.641	2.2	ng	62375	2	10.743	561760	20.0
Tetradecane	13.417	2.3	ng	91395	3	14.574	781552	20.0
n-Hexadecanoic ...	18.229	6.8	ng	341429	4	17.324	997593	20.0
Octadecanoic acid	19.504	2.6	ng	146663	5	21.584	1137030	20.0
1-Docosene	21.266	4.2	ng	240143	5	21.584	1137030	20.0